

# AI-Driven Integrated Energy Systems: Emerging Trends, Research Gaps, and Global Roadmap

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The review integrates disparate knowledge on forecasting, optimal scheduling, degradation-aware control, and resilience enhancement across power, heat, mobility, and water–energy–food nexuses, drawing on 153 recent studies covering batteries, hydrogen, thermal storage, and sector-coupled microgrids. Digital-twin and surrogate-based optimisation, deep and reinforcement learning for multi-energy dispatch, physics-informed and hybrid models, and privacy-preserving or federated analytics that respect data sovereignty while facilitating cross-asset learning are all covered by a single classification. While pointing out enduring gaps in cross-regional validation, cyber-secure implementation, and socially just deployment in vulnerable grids, the analysis quantifies typical performance gains reported for AI-enabled storage coordination, such as reductions in unmet load, curtailed renewable generation, operating cost, and emissions. Drawing from these observations, the paper lays out a three-phase global roadmap for AI-IES in energy storage from 2030 to 2050. These phases move from reliable pilots and benchmark datasets to human-centric, interoperable ecosystems and, finally, autonomous, resilience-optimized, and justice-oriented infrastructures. The roadmap provides practical advice for researchers, system operators, regulators, and investors looking to match AI innovation with net-zero, reliability, and equity targets in future integrated energy systems. It does this by connecting algorithmic decisions to technology pathways for batteries, power-to-hydrogen, long-duration storage, and hybrid storage architectures. The review offers a state-of-the-art, comprehensive basis for co-designing algorithms, market designs, and regulatory protections that expedite bankable, real-world AI-IES deployments across various regions worldwide by specifically bridging AI methodologies, storage technologies, and multi-scale planning horizons.

*Keywords: AI-driven integrated energy systems; Energy storage optimization; Digital twin; reinforcement learning; Hybrid and physics-informed AI; Multi-vector energy hubs*

## 1. Introduction

A structural change from siloed power systems to integrated energy systems that co-optimize electricity, heat, fuels, mobility, water, and digital infrastructures is being driven by the growing push for net-zero emissions, deep electrification, and sector coupling. Artificial intelligence is emerging as a key "system brain" in this transition, capable of learning multi-scale patterns, orchestrating complex assets under uncertainty,

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and ingesting heterogeneous data. The algorithmic underpinnings for next-generation integrated architectures have been laid by recent research spanning power electronics and converter-level intelligence for high-efficiency interfaces between renewables, storage, and loads [1]. Techno-economic studies on multi-vector energy hubs demonstrate how AI-coordinated scheduling can manage grid interactions, maritime logistics, and underground storage in tandem to lower system costs and curtailment while adhering to operational constraints [2]. To create early examples of AI-driven integrated energy systems, hybrid PV–fuel-cell and hydrogen infrastructures are also increasingly being built around AI-based multi-layer optimisation frameworks that coordinate generation, conversion, and storage across temporal scales [3]. Digital twins, deep learning, and IoT sensing allow for context-aware thermal comfort, adaptive control, and better building-stock renovation roadmaps, connecting device-level intelligence to district-scale efficiency and decarbonisation trajectories. Smart-building and urban studies carry this reasoning to the demand side [3-7].

In light of this, the concept of AI-Driven Integrated Energy Systems (AI-IES) refers to a converging family of architectures wherein multi-carrier infrastructures, such as district heating, microgrids, hydrogen production and refuelling corridors, water-energy-waste facilities, and electrified transportation, are closely coupled with AI, communication networks, and edge-cloud computing [8, 9]. Learning-based dispatch, forecasting, and risk management can improve flexibility and lower emissions across electricity-gas-mobility interfaces, as evidenced by recent work on hydrogen-integrated microgrids with probabilistic AI-based control, AI-optimized hydrogen refuelling stations, and AI-enabled hydrogen value chains [10]. A few examples of how distributed intelligence can integrate resilience, safety, and resource efficiency into daily operations are AI-driven smart EV charging with PV and BESS, UAV-assisted fire-hazard detection in solar plants, and smart-irrigation schemes powered by solar-IoT platforms [10]. Supporting ICT layers offer the computational and communication fabric needed for large-scale, real-time AI-IES coordination, from federated LoRaWAN architectures and 6G-ready edge AI to photonic accelerators and cloud-integrated forecasting platforms [10]. Assessments of cyber-physical vulnerabilities and smart-grid intrusion detection, which highlight the necessity of pursuing this integration with a clear focus on security, ethics, and societal risk, further support the need for a long-term, globally informed roadmap for AI-IES development over 2030–2050. [11, 12]

A more integrated literature perspective is encouraged by the fact that, despite this quickly changing landscape, existing scholarship is still dispersed along vector, scale, and disciplinary lines. Multi-vector techno-economic studies examine coordinated scheduling in particular energy hubs or corridors, such as underground storage with AI-based maritime logistics [13, 14], while power-electronics and converter-level reviews highlight AI for high-efficiency interfaces and advanced control in primarily electricity-centric settings [10]. AI mainly optimises sizing or drive-cycle energy management rather than whole-system interactions, and hybrid PV–fuel-cell and hydrogen infrastructures are frequently examined separately as grid-tied PV–FC systems or fuel-cell electric vehicles [15]. Though usually at the single-building or portfolio scale, smart-building research develops digital twins, ontologies, and deep learning for individualised comfort and asset management Nwokolo *et al.* [16]. While water-sector decarbonisation, biogas-oriented circularity, and wastewater-to-bioenergy pathways are examined within specialised WEF studies [17], parallel strands treat hydrogen microgrids, refuelling corridors, and global hydrogen systems as distinct domains [18]. In addition to ICT-centric contributions on

integrated sensing/communication/computation, 6G architectures, federated IoT, and cyber-secure smart grids [19], there is a thriving but loosely connected body of work on hybrid renewable energy systems, district heating–heat-pump portfolios, and hydrogen–biomass–PV hybrids [20, 21]. A cross-sector, cross-scale synthesis that treats AI-driven integrated energy systems as a single research program, compares AI method families and deployment architectures in a methodical manner, and disentangles long-horizon gaps—especially those related to ecosystem-scale coordination, digital-infrastructure co-design, cyber-physical risk, and the unequal representation of global South contexts—into a cohesive 2030–2050 agenda is still lacking.

In order to establish AI-Driven Integrated Energy Systems (AI-IES) as an emerging paradigm rather than a loose collection of case studies, the current study builds on this diagnosis by providing a structured, multi-layered synthesis of 153 carefully screened "critical studies". In order to connect component, asset, system, and governance layers within a single conceptual framework, the review first builds an evolutionary staging that charts the field's development from device-centric AI augmentation through asset-level intelligent facilities to fully multi-vector systems and ecosystem-scale, AI-native infrastructures [3]. Second, it creates complementary taxonomies that categorise AI-IES according to data/deployment architectures and AI method clusters, including supervised forecasting, physics-informed surrogates, digital twins, reinforcement learning, distributed edge/federated intelligence, and specialised accelerators, as well as system scope, including energy vectors, configuration topologies, and spatiotemporal scales [22]. Third, the study summarises the current use of techno-economic, resilience, flexibility, and carbon metrics in cyber-physical security frameworks, smart buildings, mobility systems, circular water-waste facilities, hydrogen and power-to-X chains, and electricity-centric systems [23]. This evidence base supports a new global roadmap for 2030–2050 that is innovative in three ways: it reframes AI-IES as an AI-native, cyber-physical ecosystem where technical architectures, governance mechanisms, and socio-environmental objectives are co-designed rather than treated as distinct optimisation problems; it explicitly couples AI, communication, and energy infrastructures; and it prioritises underserved geographies and sectors like industrial parks, agro-ecosystems, and critical-infrastructure security [24].

To convert the manuscript from a linear narrative into a staged knowledge pipeline for AI-Driven Integrated Energy Systems (IES), Table 1 summarises the general architecture of the review, mapping each major section to its primary goal and the particular results it produces. By clearly connecting methodological underpinnings to the comparative typology analysis, multi-axis classification framework, and the 2030–2050 roadmap, Table 1 makes it clear how evidence is gradually sorted, filtered, and then projected into useful insights. Further illustrating how technical, economic, environmental, governance, and just-transition aspects are integrated rather than addressed separately is the inclusion of special sections on new trends, research gaps, and structured policy pillars.

**Table 1.** Structure and focus of the review

| Section                                            | Purpose                                                                                                                                | What it achieves                                                                                                                                                                                     |
|----------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 2. Methodology                                     | To formalise the systematic review and mixed bibliometric–content analysis protocol used to construct the AI-Driven IES evidence base. | Delivers a transparent, reproducible pipeline for identifying, filtering, and synthesising 2019–2025 AI-Driven IES studies across energy, ICT, transport, buildings, industry, and hydrogen systems. |
| 3. Current Research Status of AI-Driven Integrated | To characterise the global publication landscape (annual output, countries,                                                            | Highlights acceleration in AI-IES publications, identifies regional and disciplinary hotspots, and                                                                                                   |

|                                                                                                       |                                                                                                                                                                                                              |                                                                                                                                                                                                         |
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| Energy Systems                                                                                        | sources, and subject areas) for AI-Driven IES.                                                                                                                                                               | exposes under-represented geographies and domains that inform later gap analysis and roadmap design.                                                                                                    |
| 4. Evolutionary stages of AI-Driven Integrated Energy Systems studies                                 | To reconstruct how AI-IES research has evolved from single-vector optimisation to multi-vector, cyber-physical, and digital-twin-enabled systems.                                                            | Provides a temporal scaffold (early component-level control, hybrid microgrids, sector-coupled infrastructures, and DT-orchestrated ecosystems) that underpins the staged 2030–2050 global roadmap.     |
| 5. Classification of AI-Driven Integrated Energy Systems                                              | To introduce an overarching classification framework that organises AI-IES studies along system, resource, application, and digitalisation axes.                                                             | Unifies heterogeneous case studies into a single conceptual space, enabling cross-study comparison and identification of neglected combinations of vectors, scales, and AI roles.                       |
| 5.1 System-scope classification by energy vectors, configuration, and spatio-temporal scale           | To distinguish IES by the number and type of coupled energy carriers (electricity, heat, hydrogen, fuels, water), configuration (on/off-grid, prosumer, industrial park), and temporal/spatial scale.        | Clarifies how AI tasks, data requirements, and control horizons change from device- and building-scale systems to regional, cross-border, and multi-sector platforms.                                   |
| 5.2 Resource-scale classification for AI-Driven IES applications                                      | To classify systems according to primary resources and conversion chains (solar–PV, wind, biomass, geothermal, waste heat, water–energy nexus, etc.).                                                        | Reveals which resource couplings (e.g., PV–wind–H <sub>2</sub> , waste-heat–district heating, desalination–renewables) have rich AI coverage and which remain under-explored.                           |
| 5.3 Application-scale classification of AI-Driven integrated energy systems                           | To group AI-IES studies by end-use context (buildings and campuses, manufacturing, mobility and EV/FCV infrastructure, smart cities, data centres, ports, and agro-energy systems).                          | Links AI-driven integration patterns to sector-specific constraints and opportunities, enabling targeted replication of promising architectures across domains.                                         |
| 5.4 Digital-twin and cyber–physical classification for AI-Driven IES                                  | To differentiate levels of digitalisation, from offline forecasting and planning to closed-loop digital twins with real-time sensing, control, and optimisation.                                             | Establishes maturity tiers for AI-IES digital infrastructures, clarifying the gap between current pilot-scale DT deployments and fully cyber-physical, grid-interactive energy ecosystems.              |
| 5.5 Performance-indicator classification for AI-Driven IES                                            | To organise the diverse metrics used to evaluate AI-Driven IES into coherent families (technical, economic, environmental, flexibility, reliability/resilience, cybersecurity, equity and governance).       | Provides a multi-criteria evaluation lens that goes beyond cost and efficiency, enabling balanced assessment of AI-IES impacts on reliability, emissions, social justice, and institutional robustness. |
| 6. Comparative Analysis of AI-Driven Integrated Energy Systems Typologies and Optimization Strategies | To cross-tabulate IES typologies with the AI and optimisation strategies used (e.g., deep learning, reinforcement learning, metaheuristics, MPC, hybrid controllers).                                        | Identifies which AI methods are most frequently and effectively paired with specific IES configurations and objectives, and where methodological mismatches or blind spots persist.                     |
| 6.1 Typologies of AI-Driven Integrated Energy Systems                                                 | To synthesise recurring AI-IES archetypes (e.g., PV–battery–EV microgrids, hydrogen-integrated industrial clusters, smart buildings with DTs, district heating with heat pumps, 6G-enabled energy services). | Generates a library of transferable design patterns that can be adapted by planners, utilities, and policymakers when architecting future AI-powered integrated systems.                                |
| 6.2 Optimization and control strategies across typologies                                             | To compare how different IES typologies implement AI-driven forecasting, scheduling, dispatch, and real-time control strategies.                                                                             | Illuminates trade-offs between centralised cloud optimisation and edge/embedded intelligence, offline versus online learning, and single-objective versus multi-objective control in complex IES.       |
| 6.3 Proposed Conceptual Taxonomy for AI-Driven Integrated Energy Systems                              | To integrate system-scope, resource, application, digital-twin maturity, AI method families, and performance indicators into a single conceptual taxonomy.                                                   | Delivers a reusable classification blueprint that future studies can adopt to position new AI-IES designs consistently and to benchmark them against the existing global corpus.                        |
| 7 Key Findings and Implications across AI-Driven IES                                                  | To synthesise cross-cutting findings from the classifications, typologies, and optimisation analyses into high-level lessons.                                                                                | Distils system design principles, methodological best practices, and priority research and policy themes that directly inform the roadmap and policy pillars.                                           |
| 8. Emerging trends, research gaps, and global roadmaps (2030–2050)                                    | To align observed trajectories in AI methods, digital infrastructures, sectoral applications, and governance debates with a forward-looking 2030–2050 agenda.                                                | Connects empirical evidence to a staged global roadmap, ensuring that proposed milestones for AI-Driven IES are grounded in current capabilities while stretching toward transformative futures.        |
| 8.1 Emerging trends and                                                                               | To articulate dominant technological                                                                                                                                                                         | Provides a structured gap analysis that pinpoints                                                                                                                                                       |

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| research gaps in AI-Driven integrated energy systems                   | and socio-technical trends and to isolate persistent gaps in data, models, infrastructure, and institutions.                                                                                                     | where targeted research, demonstration, and capacity-building efforts are most needed in the coming decade.                                                                            |
| 8.2 Global roadmap for AI-Driven integrated energy systems (2030–2050) | To translate trends and gaps into a three-phase roadmap: foundations and pilots (2026–2030), scaled and interoperable human-centric systems (2030–2040), and autonomous, resilient, and just AI-IES (2040–2050). | Offers a time-phased, globally relevant pathway that links near-term research and demonstration to long-term deployment, regulatory evolution, and just transition objectives.         |
| 9. Conclusions and Policy Recommendations                              | To consolidate the review’s insights into concise messages for researchers, industry, regulators, and international organisations.                                                                               | Bridges scientific synthesis and actionable guidance, framing AI-Driven IES as both a technological and governance challenge that must be addressed through coordinated policy action. |

## 2. Methodology

### 2.1 Search Strategy

The search strategy aimed to identify cutting-edge applications of artificial intelligence in integrated energy systems (IES) by amalgamating a comprehensive array of multi-energy system descriptors with an extensive block of AI and data-driven methodologies, subsequently adapting this framework to the syntax of each database. Six principal platforms were examined: Scopus, Web of Science Core Collection, Google Scholar, ScienceDirect, Taylor & Francis Online, and SpringerLink. These were chosen to ensure a comprehensive bibliographic scope (Scopus, Web of Science), robust coverage of energy and engineering journals (ScienceDirect, Taylor & Francis Online, SpringerLink), and further exploration via citation chaining and conference proceedings (Google Scholar). In each database, search queries integrated two idea clusters utilising Boolean logic: (i) an IES/system block and (ii) an AI/method block. The IES block encompassed terminology including “integrated energy system”, “multi-energy system”, “multi-carrier energy”, “sector-coupled energy”, “energy hub”, “hybrid renewable energy system”, “microgrid”, and “smart grid” to guarantee representation of electricity, heat, gas, hydrogen, and storage integrations. The AI block included terms such as “artificial intelligence”, “AI-driven”, “data-driven”, “machine learning”, “deep learning”, “reinforcement learning”, “graph neural network”, “digital twin”, “physics-informed”, “metaheuristic”, “evolutionary algorithm”, “genetic algorithm”, “particle swarm”, “Bayesian optimisation”, and “surrogate model” to represent the contemporary toolkit utilised for IES planning, control, and optimisation. The publication period was limited to 2019–2025 across all databases using year filters or specific date ranges. The lower bound of 2019 was selected to emphasize the latest generation of AI-driven IES research, aligning with the swift advent of deep learning, reinforcement learning, digital-twin architectures, graph neural networks, and physics-informed models inside multi-energy frameworks. The maximum limit (2025) is the most recent complete period available during the search, guaranteeing the inclusion of early-access and in-press research where permitted by the databases. Further filters were implemented to limit results to peer-reviewed journal articles, significant conference papers, and review articles in energy, power systems, smart grids, and associated engineering fields, thus ensuring the final corpus aligns with the methodological and thematic framework of the AI-Driven Integrated Energy Systems study [25–29].

**Table 2.** Database-specific search strategy table tailored to AI-Driven Integrated Energy Systems (IES)

| Database                         | Search query (2019–2025)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        | Additional filters                                                                                                                           | Justification/focus (AI-Driven IES, 2019–2025)                                                                                                                                                                                                                                                                                                                                                      |
|----------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Scopus                           | TITLE-ABS-KEY( "integrated energy system*" OR "multi-energy system*" OR "multi energy system*" OR "multi-vector energy system*" OR "multi vector energy" OR "multi-carrier energy" OR "sector-coupled energy" OR "energy hub*" OR "hybrid renewable energy system*" OR "hybrid energy system*" OR microgrid* OR "smart grid" ) AND TITLE-ABS-KEY( "artificial intelligence" OR "AI-driven" OR "AI based" OR "data-driven" OR "machine learning" OR "deep learning" OR "reinforcement learning" OR "transfer learning" OR "graph neural network*" OR "convolutional neural network*" OR "digital twin" OR "physics-informed" OR metaheuristic* OR "evolutionary algorithm*" OR "genetic algorithm*" OR "particle swarm" OR "bayesian optimization" OR "surrogate model*" ) AND PUBYEAR > 2018 AND PUBYEAR < 2026 | - Years: 2019–2025 (via PUBYEAR > 2018 AND < 2026) - Doc type: Article, Review - Language: English                                           | Uses TITLE-ABS-KEY to capture the core IES concepts (multi-energy/sector-coupled systems, energy hubs, hybrid RES, microgrids, smart grids) plus advanced AI enablers (DL, RL, GNNs, digital twins, metaheuristics, Bayesian optimisation). The 2019–2025 window focuses on the latest AI wave and aligns with an IES manuscript centred on next-generation control, optimisation, and forecasting. |
| Web of Science (Core Collection) | TS=( ("integrated energy system*" OR "multi-energy system*" OR "multi energy system*" OR "multi-vector energy system*" OR "multi vector energy" OR "multi-carrier energy" OR "sector-coupled energy" OR "energy hub*" OR "hybrid renewable energy system*" OR "hybrid energy system*" OR microgrid* OR "smart grid") AND ("artificial intelligence" OR "AI-driven" OR "AI based" OR "data-driven" OR "machine learning" OR "deep learning" OR "reinforcement learning" OR "transfer learning" OR "graph neural network*" OR "convolutional neural network*" OR "digital twin" OR "physics-informed" OR metaheuristic* OR "evolutionary algorithm*" OR "genetic algorithm*" OR "particle swarm" OR "bayesian optimization" OR "surrogate model*") ) AND PY=(2019-2025)                                           | - Timespan: 2019–2025 - Doc type: Article, Review - Indexes (typical): SCI-EXPANDED, SSCI                                                    | TS (Topic) searches title, abstract, and keywords, making it ideal for a structured concept block. The query fuses integrated/multi-energy infrastructure terms with a rich AI toolbox reflective of 2019–2025 practice (digital twins, physics-informed models, GNNs, RL). This yields a focused corpus on AI-driven IES planning, operation, and resilience.                                      |
| Google Scholar                   | ("integrated energy system" OR "multi-energy system" OR "multi energy system" OR "multi-vector energy system" OR "multi vector energy" OR "sector-coupled energy" OR "multi-carrier energy" OR "energy hub" OR "hybrid renewable energy system" OR "hybrid energy system" OR microgrid OR "smart grid") AND ("artificial intelligence" OR "AI driven" OR "AI based" OR "data driven" OR "machine learning" OR "deep learning" OR "reinforcement learning" OR "graph neural network" OR "digital twin" OR "physics-informed" OR metaheuristic OR "evolutionary algorithm" OR "genetic algorithm" OR "particle swarm" OR "bayesian optimization" OR "surrogate model") then set Custom range: 2019–2025                                                                                                           | - Date range: 2019–2025 (Custom range) - Sort by relevance - Optionally add review to find surveys                                           | Scholar lacks fielded searching, so a free-text Boolean query is used, with a strong IES concept block plus an expanded modern AI block (including digital twin, GNN, physics-informed, surrogate modelling). The 2019–2025 filter emphasises contemporary AI-powered IES work in journals, theses, and conferences, matching the manuscript's cutting-edge scope.                                  |
| ScienceDirect                    | TITLE-ABSTR-KEY( "integrated energy system*" OR "multi-energy system*" OR "multi energy system*" OR "multi-vector energy system*" OR "multi vector energy" OR "sector-coupled energy" OR "multi-carrier energy" OR "energy hub*" OR "hybrid renewable energy system*" OR "hybrid energy system*" OR microgrid* OR "smart grid" ) AND TITLE-ABSTR-KEY( "artificial intelligence" OR "AI-driven" OR "AI based" OR "data-driven" OR "machine learning" OR "deep learning" OR "reinforcement learning" OR "graph neural network*" OR "digital twin" OR "physics-informed" OR metaheuristic* OR "evolutionary algorithm*" OR "genetic algorithm*" OR "particle swarm" OR "bayesian optimization" OR "surrogate model*" ) then limit to 2019–2025                                                                     | - Years: 2019–2025 - Article type: Research Articles, Review Articles - Subject areas: Energy, Engineering, Computer Science (optional)      | ScienceDirect hosts key energy and power systems journals. Restricting to TITLE-ABSTR-KEY yields high precision for AI-enhanced IES (e.g., hybrid PV–wind–storage hubs, power-heat-gas couplings, hydrogen-linked IES). The AI block includes post-2019 methods such as digital twins and physics-informed learning, matching a state-of-the-art AI-driven IES review.                              |
| Taylor & Francis Online          | Advanced Search, “in: Title, Abstract, Keywords”: ("integrated energy system*" OR "multi-energy system*" OR "multi energy system*" OR "multi-vector energy system*" OR "multi vector energy" OR "multi-carrier energy" OR "sector-coupled energy" OR "energy hub*" OR "hybrid renewable energy system*" OR "hybrid energy system*" OR microgrid* OR "smart grid") AND ("artificial intelligence" OR "AI-driven" OR "AI based" OR "data-driven" OR "machine learning" OR "deep learning" OR "reinforcement learning" OR "graph neural network*" OR "digital twin" OR "physics-informed" OR metaheuristic* OR "evolutionary algorithm*" OR "genetic algorithm*" OR "particle swarm" OR "bayesian optimization" OR "surrogate model*") then set 2019–2025                                                          | - Publication date: 2019–2025 - Content type: Research article, Review article - Subject: Engineering, Energy, Environment, Computer Science | Taylor & Francis carries influential energy and optimisation titles. Limiting search to Title/Abstract/Keywords removes generic AI or generic energy work, surfacing studies that explicitly position AI as the driver of IES design, scheduling, or control in the 2019–2025 period. This is well aligned with a focused AI-Driven IES manuscript.                                                 |
| SpringerLink                     | ("integrated energy system*" OR "multi-energy system*" OR "multi                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | - Years: 2019–                                                                                                                               | SpringerLink is rich in smart-grid,                                                                                                                                                                                                                                                                                                                                                                 |

|  |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |                                                                                                                   |                                                                                                                                                                                                                                                                                                                                                                |
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|  | energy system*" OR "multi-vector energy system*" OR "multi vector energy" OR "multi-carrier energy" OR "sector-coupled energy" OR "energy hub*" OR "hybrid renewable energy system*" OR "hybrid energy system*" OR microgrid* OR "smart grid") AND ("artificial intelligence" OR "AI-driven" OR "AI based" OR "data-driven" OR "machine learning" OR "deep learning" OR "reinforcement learning" OR "graph neural network*" OR "digital twin" OR "physics-informed" OR metaheuristic* OR "evolutionary algorithm*" OR "genetic algorithm*" OR "particle swarm" OR "bayesian optimization" OR "surrogate model*") then filter Content type = Article, Chapter and Year: 2019–2025 | 2025 - Content type: Journal Article, Book Chapter - Disciplines (optional): Energy, Engineering, Smart Grids, AI | multi-carrier energy, and digital-twin research. The query targets integrated/multi-energy infrastructures plus an extended AI block that captures the latest algorithmic and DT developments. Limiting to 2019–2025 focuses the evidence base on recent deployments of AI-driven IES, including urban energy hubs and sector-coupled power-gas-heat networks. |
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## 2.2 Study Selection and Screening

Records retrieved from Scopus, Web of Science, Google Scholar, ScienceDirect, Taylor & Francis Online, and SpringerLink were first de-duplicated and then passed through a two-stage screening pipeline: (i) title–abstract screening and (ii) full-text eligibility assessment. At each stage, predefined inclusion approaches (IA1–IA5) and exclusion approaches (EA1–EA6) were applied to ensure conceptual alignment with AI-Driven IES and methodological robustness. During title–abstract screening, records were retained only if they explicitly referred to integrated, multi-energy, or sector-coupled configurations rather than isolated technologies (IA1), and if AI, machine learning, or advanced data-driven methods were clearly positioned as a central enabler for planning, control, or optimization of the system (IA2). The screening form required at least one unambiguous cue from both the “system” block and the “AI” block. For the system dimension, reviewers looked for terms such as integrated energy system, multi-energy system, multi-carrier energy hub, sector-coupled, hybrid renewable energy system, or microgrid with combined power–heat–gas or power–H<sub>2</sub> couplings. For the AI dimension, reviewers flagged phrases such as 'AI-driven optimisation', 'machine learning-based dispatch', 'deep reinforcement learning for multi-energy scheduling', 'digital twin of integrated energy hub', or 'metaheuristic AI sizing of hybrid systems'. Records that clearly described only single-technology optimisation (PV MPPT, stand-alone wind turbine control, or battery state-of-charge prediction) without multi-carrier or integrated context were excluded at this stage under EA1, while studies relying solely on classical deterministic optimization without any AI or data-driven component were removed under EA2. In parallel, temporal and publication-type constraints were applied consistently across databases. Only studies with a publication year between 2019 and 2025 were considered eligible (IA4); any record outside this range was excluded irrespective of topical relevance (EA3). This temporal focus was chosen to capture the most recent wave of developments in deep learning, reinforcement learning, digital twins, graph neural networks, and physics-informed models as they began to be systematically embedded in IES architectures. Furthermore, only peer-reviewed research articles, substantial review papers, and full conference contributions in energy, power systems, smart grids, or related engineering domains were retained (IA5). Editorials, commentaries, news items, book reviews, white papers, and other grey literature were excluded under EA4 to maintain a high and consistent methodological quality threshold. At the full-text screening stage, the same inclusion and exclusion logic was operationalized with greater granularity. Studies were included only if they reported system-level performance or design outcomes relevant to integrated energy systems—such as levelised cost of energy or hydrogen (LCOE, LCOH), net present cost, renewable penetration, flexibility indices,

hosting capacity, reliability metrics, resilience indicators, or emissions reductions (IA3). Full texts that mentioned AI and IES but remained purely conceptual, policy-oriented, or narrative without presenting explicit models, architectures, algorithms, or quantitative evaluation were excluded under EA6. Likewise, studies where AI was deployed in tangential domains—such as vehicle styling, social media analytics, or generic computer vision—without clear modelling, operation, or planning of integrated energy infrastructures were screened out under EA5. By enforcing these criteria, the final corpus was restricted to quantitatively grounded, AI-driven studies that directly interrogate the design, control, or optimization of multi-carrier, sector-coupled, or hybrid renewable energy systems, thereby ensuring strong alignment with the core scope and objectives of the AI-Driven Integrated Energy Systems manuscript [30-36].

**Table 3.** Inclusion Approaches and Exclusion Approaches tailored to an AI-Driven Integrated Energy Systems (IES)

| Code | Inclusion / Exclusion statement                                                                                                               | How to operationalize during screening                                                                                                                                                                                                                                                                  | Example cues aligned with the manuscript                                                                                                                                                                                         | Why this aligns with IES                                                                                                                                                                                |
|------|-----------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| IA1  | Studies must explicitly address integrated or multi-energy systems rather than single isolated technologies.                                  | At title/abstract level, include only records that mention integrated/multi-energy/multi-vector systems, sector coupling, energy hubs, hybrid multi-carrier systems, or microgrids with explicit coupling of at least two carriers (e.g., power–heat, power–gas, power–H <sub>2</sub> , power–storage). | Phrases such as “integrated energy system”, “multi-energy system”, “sector-coupled energy”, “multi-carrier energy hub”, “hybrid PV–wind–battery–H <sub>2</sub> system”, “microgrid with combined heat and power”.                | IES is inherently about coupled energy carriers and infrastructures; this criterion ensures the corpus reflects system-level integration, not isolated components.                                      |
| IA2  | Studies must employ AI, machine learning, or advanced data-driven methods as a central enabler for IES planning, control, or optimization.    | During abstract/full-text screening, retain papers where AI/ML is a core methodological element for IES (not just a passing mention). Check methods and keywords for explicit AI algorithms and data-driven modelling.                                                                                  | Terms including “artificial intelligence”, “AI-driven”, “machine learning”, “deep learning”, “reinforcement learning”, “digital twin”, “graph neural network”, “metaheuristic AI optimizer”, “surrogate-based learning for IES”. | The manuscript focuses on AI-Driven IES; this criterion filters to studies where AI is not peripheral but drives dispatch, sizing, coordination, forecasting, or co-optimization of integrated systems. |
| IA3  | Studies must report system-level performance or design outcomes relevant to IES (e.g., techno-economic, reliability, flexibility, emissions). | Include papers that quantify impacts at system level: LCOE, LCOH, NPC, cost savings, renewable penetration, resilience indices, emission reductions, flexibility/reserve metrics, or hosting capacity. Exclude purely conceptual AI/algorithm papers with no applied IES metrics.                       | Phrases such as “optimal sizing of multi-energy hub”, “cost–emissions trade-off for integrated system”, “improved reliability index for AI-controlled microgrid”, “GHG reduction in AI-optimised hybrid system”.                 | AI-Driven IES research is impactful when it changes system behaviour or outcomes; this criterion prioritises quantifiable benefits and trade-offs central to IES design and operation.                  |
| IA4  | Studies must fall within the publication window 2019–2025 to reflect the latest AI and digital-twin advances.                                 | Use database filters to restrict years to 2019–2025. At screening, exclude any record with publication year <2019 or >2025, even if conceptually relevant.                                                                                                                                              | Metadata showing “Published: 2020”, “First online: 2022” etc.; database year filters set to 2019–2025.                                                                                                                           | The AI-Driven IES field accelerated after ~2019 with deep learning, RL, digital twins, and physics-informed models; this window captures the state-of-the-art that the manuscript aims to synthesise.   |
| IA5  | Studies must be peer-reviewed full research articles or substantial reviews in energy/engineering/related domains.                            | Check document type; include journal articles and substantial conference papers/review articles. Exclude editorials, notes, book reviews, non-reviewed reports, and short news pieces.                                                                                                                  | Document types labelled “Article”, “Research Article”, “Review”, “Full conference paper” in energy, power systems, smart grids, renewables, or related engineering fields.                                                       | Peer-reviewed research provides robust, validated evidence for AI-Driven IES, ensuring that the synthesis rests on methodologically sound contributions.                                                |
| EA1  | Exclude single-technology studies without system integration (e.g., stand-alone PV, battery, or wind AI control without multi-                | At title/abstract level, screen out papers focusing solely on one asset (PV, WT, battery, PEMFC) where there is no integration with other carriers or loads at system                                                                                                                                   | Phrases like “MPPT for PV array”, “fault diagnosis in wind turbine gearbox”, “battery SOC prediction” without terms such as multi-energy, energy hub, CHP,                                                                       | Such work, while valuable, does not capture interactions across energy carriers that define IES; keeping it would dilute the system-integration                                                         |

|     | energy coupling).                                                                                                                                                      | level.                                                                                                                                                                                  | sector coupling, etc.                                                                                                                                                                          | focus of the manuscript.                                                                                                                                                              |
|-----|------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| EA2 | Exclude studies that do not use AI, ML, or advanced data-driven methods as a core methodology (e.g., purely deterministic or classical optimization only).             | Discard papers where methods rely solely on linear programming, MILP, classical optimal power flow, or rule-based control with no AI/ML or data-driven layer.                           | Methods sections dominated by “MILP optimization”, “deterministic optimal dispatch”, “rule-based control” without AI keywords like ML, DL, RL, digital twin, metaheuristics framed as AI.      | The review’s distinctive value lies in AI-driven approaches; purely conventional optimization lacks this AI layer and therefore sits outside the central research question.           |
| EA3 | Exclude studies outside the 2019–2025 time window.                                                                                                                     | Apply strict year filters and remove records with publication year prior to 2019 or after 2025 during screening, even if thematically relevant.                                         | Any record tagged as 2010, 2014, 2017, or future-early-access beyond 2025.                                                                                                                     | Earlier work predates the surge of deep AI integration and digital twins in IES; including it would blur the focus on the most recent technological wave.                             |
| EA4 | Exclude non-peer-reviewed, grey, or informal literature (reports, theses without journal publication, white papers, websites).                                         | Identify and remove entries sourced from repositories, non-reviewed reports, project deliverables, or institutional websites that do not indicate peer review.                          | Items tagged as “technical report”, “white paper”, “working paper”, institutional PDFs without journal details, or generic web pages.                                                          | Maintaining a peer-reviewed evidence base ensures consistency in methodological quality and credibility, which is crucial for a high-impact AI-Driven IES synthesis.                  |
| EA5 | Exclude studies where AI is applied outside the energy-system/IES domain (e.g., vehicle styling, social media, generic computer vision) even if “energy” is mentioned. | During abstract screening, remove papers where AI is used for tangential tasks (design aesthetics, driver behaviour, marketing) with no explicit IES modelling, operation, or planning. | Examples: “deep learning for EV body styling”, “AI sentiment analysis for energy policy debates”, “GANs for battery image segmentation without system context”.                                | The manuscript is centred on AI as an operational/intelligence layer for IES, not on general AI applications; tangential domains dilute thematic coherence.                           |
| EA6 | Exclude purely conceptual/policy papers that lack explicit models, architectures, or quantitative evaluation of AI-Driven IES.                                         | At full-text stage, exclude documents that discuss AI and IES mostly at narrative or policy level without presenting models, architectures, algorithms, or numerical results.           | Phrases like “conceptual framework for AI in energy transition”, “narrative review of AI and policy” with no equations, algorithms, or simulation/experimental results for integrated systems. | The review aims to synthesise model-based, computational, and quantitative evidence for AI-Driven IES; purely discursive work cannot support system-level methodological conclusions. |

### 2.3 Study refinement and integration workflow

The study refinement and integration workflow for the AI-driven integrated energy systems (IES) review follows a multi-stage funnel that progressively concentrates the evidence base from a broad discovery set into a tightly curated corpus of critical studies. Initial identification yielded 323 records from Scopus, Web of Science, Google Scholar, ScienceDirect, Taylor & Francis Online, and SpringerLink, using qualification searches limited to peer-reviewed English-language documents. Automated de-duplication in Mendeley removed 34 overlapping entries, leaving 289 unique studies that entered the screening phase. These were screened against inclusion approaches IA1–IA5, which enforce integrated or multi-energy system scope, explicit AI/data-driven methodology, system-level performance outcomes, the 2019–2025 publication window, and peer-reviewed status. Manual application of exclusion approaches EA1 and EA2 at this stage removed 23 single-technology or non-AI papers, while EA3 and EA4 eliminated a further 18 records that failed temporal or quality thresholds, yielding 248 studies for full-text eligibility assessment. Detailed full-text review, guided by EA5 and EA6, excluded 34 studies that used AI outside the IES domain or remained purely conceptual/policy-oriented without quantitative models, leaving 214 core articles. To avoid missing influential contributions, a snowballing step added 7 further records from reference lists, after which all 221 candidates were re-tested against the full IA/EA set, leading to the removal of 56 additional studies that did not consistently satisfy integrated,

AI-driven, and quantitative IES criteria. This produced 165 studies included for in-depth analysis.

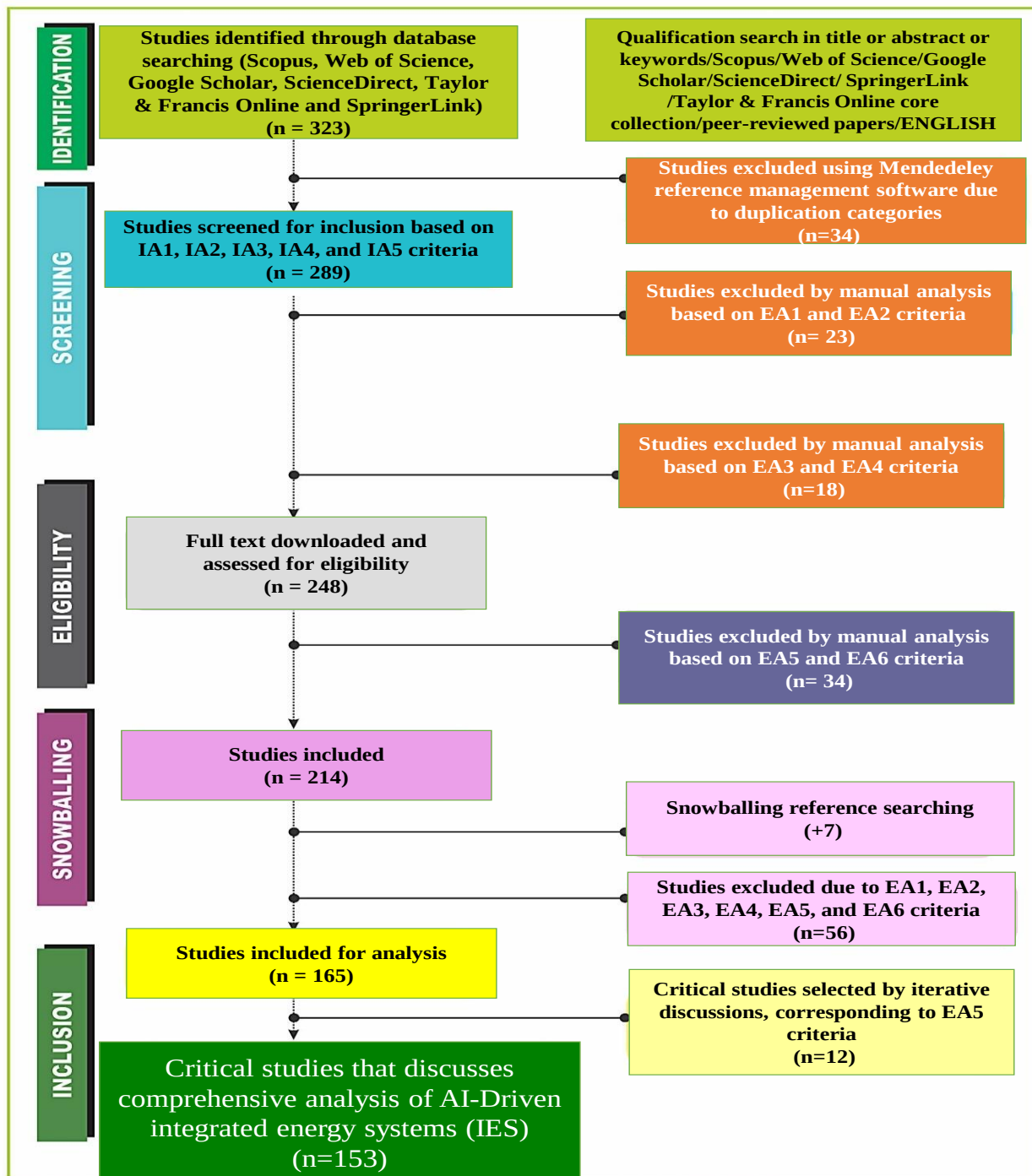


Fig. 1. Study refinement and integration workflow

### 3. Current Research Status

The current research landscape on AI-driven integrated energy systems (IES) is clearly in an exponential take-off phase: annual publications climb from a single paper in 2019 to 4–8 studies per year between 2020 and 2023, before surging to 27 in 2024 and 104 in 2025, meaning almost 70% of all 153 retrieved documents were published in 2025 alone, a typical signature of a rapidly consolidating emerging field, as shown in Fig. 2a. A geographically diverse but strongly Asia-led ecosystem supports this growth: China and India together contribute well over one-third of all outputs ( $\approx 34$  and  $\approx 29$  papers, respectively), followed by a second tier of producers—including the United States, Italy, Spain, Saudi Arabia, the United Kingdom, Malaysia, South Korea, Germany, and Canada—each with roughly 8–18 publications, and a long tail of countries in Europe, the Middle East, Africa, and Latin America with 2–6 documents apiece, indicating that AI-IES concepts are no longer confined to a few technology frontrunners but are being stress-tested in very different grid, climate, and socio-economic contexts, as shown in Fig. 2b. The journal and source profile reinforces this dual pattern of consolidation and dispersion: IEEE Access stands out with about 10 papers, while *Energies* and major energy and hydrogen outlets such as *Applied Energy*, *International Journal of Hydrogen Energy*, *Journal of Building Engineering*, *Scientific Reports*, and *Chemical Engineering Journal* each host around five articles, and a diverse cluster of specialized venues—including *Energy*, *Engineering Applications of Artificial Intelligence*, *IEEE Internet of Things Journal*, *Journal of Energy Storage*, *Journal of Environmental Management*, *Sustainable Energy Grids and Networks*, and *Sustainable Energy Technologies and Assessments*—carry 2–3 papers each, signaling that AI-IES research is simultaneously embedded in mainstream power/energy journals and in AI, IoT, and sustainability-oriented platforms, as shown in Fig. 2c. Finally, the subject-area distribution shows that the field is structurally interdisciplinary but firmly anchored in engineering and computation: engineering accounts for more than half of the documents ( $\approx 89$ ); computer science and energy each contribute on the order of 46–49 papers; while environmental science, materials science, physics and astronomy, mathematics, chemical engineering and chemistry add smaller but non-trivial shares, with a residual presence in earth and planetary sciences and biochemistry, as shown in Fig. 2d [37–42].

The current research status of AI-driven integrated energy systems (IES) revealed by panels (e)–(g) shows a strongly international but thematically coherent community concentrated around a small set of highly active institutions, funders, and authors. At the institutional level (Fig. e), Prince Sattam Bin Abdulaziz University leads with five publications, while Nanyang Technological University and King Khalid University follow with four each, and a second tier of globally distributed universities—including Heriot-Watt University, Tsinghua University, Huazhong University of Science and Technology, Jouf University, INTI International University, Saveetha School of Engineering, Saveetha Institute of Medical and Technical Sciences, and the University of Tabuk—each contribute three papers, signaling a dense nexus of activity spanning Saudi Arabia, East and Southeast Asia, the UK, and India. Funding distribution (Fig. 3f) confirms that AI-driven IES is increasingly seen as strategic infrastructure research: the National Natural Science Foundation of China underpins the field with ten funded studies, complemented by the National Key Research and Development Program of China (seven publications), the U.S. National Science Foundation (five), and major multi-country programmes such as Horizon 2020 and Horizon Europe, alongside national and

institutional sponsors including King Khalid University, the National Research Foundation of Korea, the U.S. Department of Energy, China Scholarship Council, the

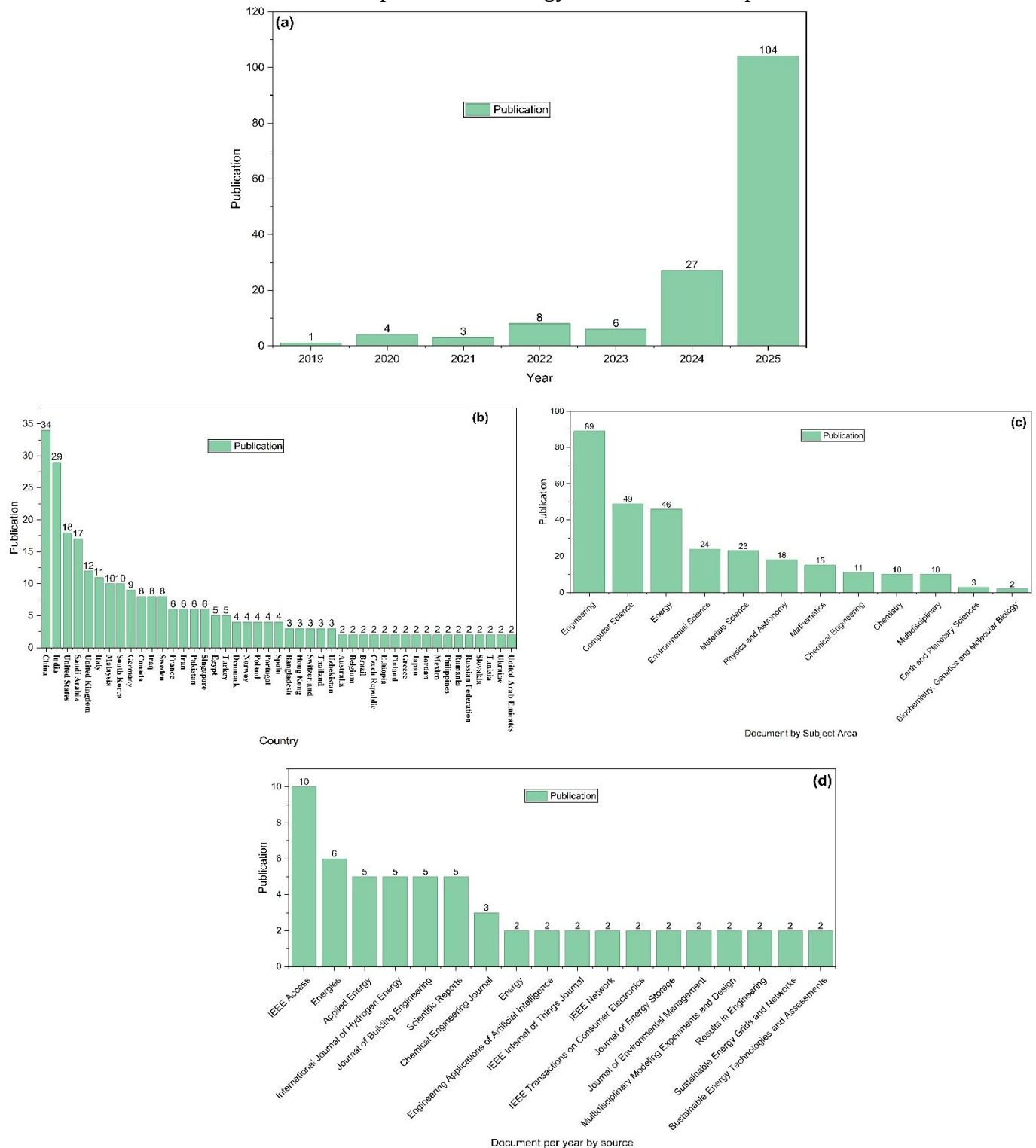


**Fig. 2.** Current research status of the revealed AI-driven integrated energy system (IES). (a) Number of annual publications, (b) Document by Country, (c) Document per year by source, (d) Research domain distribution (subject area)

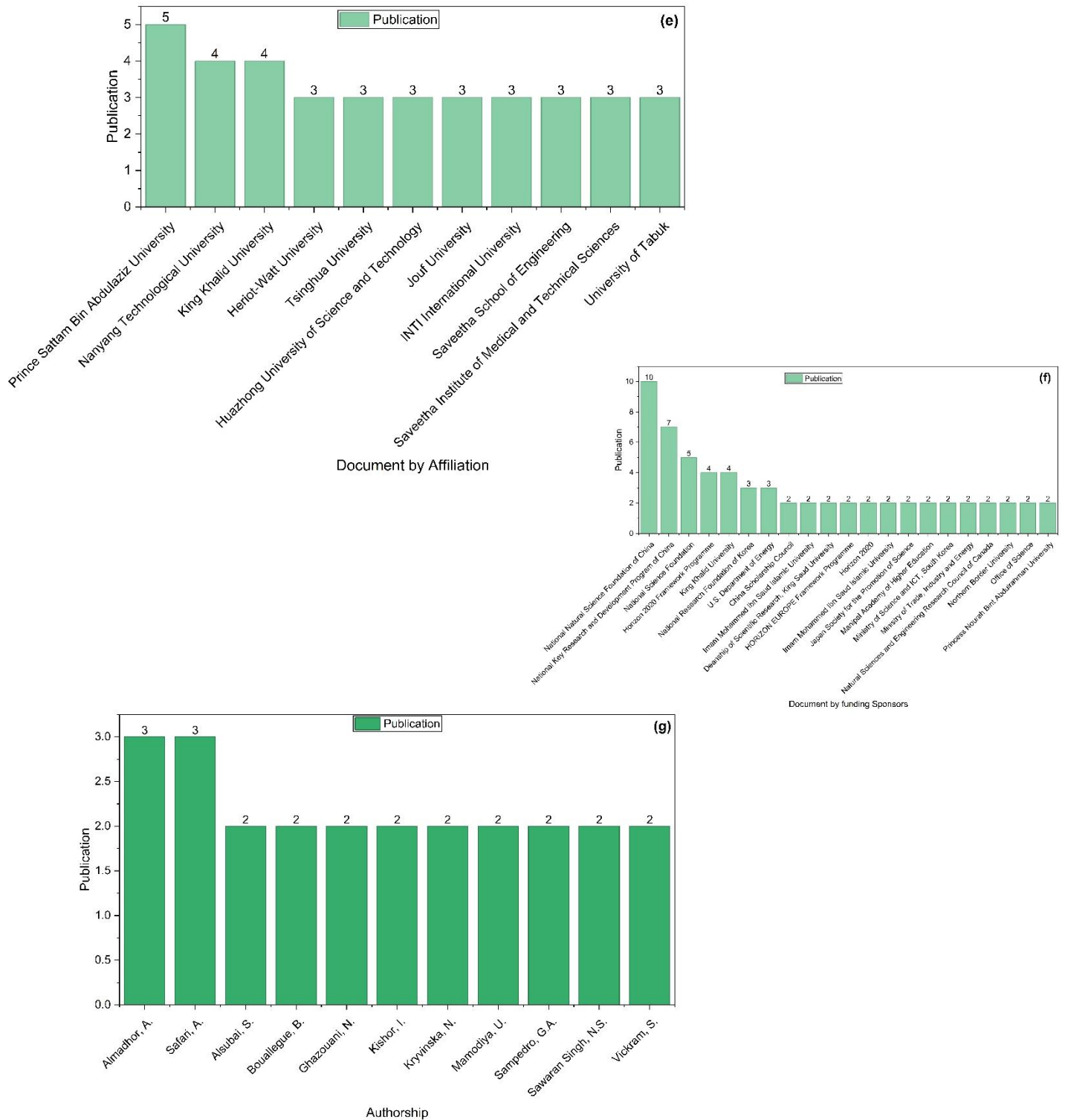


**Fig. 3.** Current research status of the revealed AI-driven integrated energy system (IES). (e) Document by affiliation, (f) Funding sponsors distribution, and (g) Document by authorship

Japan Society for the Promotion of Science, the Ministry of Science and ICT (South Korea), the Natural Sciences and Engineering Research Council of Canada, and several Saudi university deanships. Authorship patterns (Fig. 3g) show a moderate concentration of expertise rather than dominance by a single research group: [43] each contribute three papers, while [43-48] contribute two each, suggesting a distributed leadership structure where multiple teams are independently pushing the frontier on AI-enabled planning, optimisation, and control of multi-energy, sector-coupled systems. Together, these affiliation–funding–authorship patterns indicate that AI-driven IES has moved beyond isolated case studies into a globally networked research domain anchored by strong national science agencies and cross-continental collaborations, positioning the field for rapid methodological maturation and large-scale deployment.

#### 4. Evolutionary Stages of AI-Driven Integrated Energy Systems Studies

The 153-study corpus is synthesized in Table 4 and Fig. 4 into a logical evolutionary trajectory that starts with component-centric AI applications and progressively moves towards fully integrated energy–information ecosystems. Efforts to use neural networks and pattern-recognition frameworks to approximate complex device physics and control behaviour define the earliest stage. The simulation and optimisation of adsorption chillers in combined heating and cooling systems serve as evidence that neural networks can effectively capture nonlinear thermodynamic responses at the component scale [49]. Similar to this, structural elements are treated as self-powered sensing units in machine-learning-based damage identification using harvested-energy variations, which predicts subsequent condition-monitoring strategies in larger networks [50]. Prognostics and health management for marine hybrid energy systems serve as examples of how data-driven models can optimise operating schedules under uncertainty and extend asset lifetimes [51]. Parallel to this, the shift from classical control to AI-enhanced schemes for power-electronics interfaces is reflected in the adaptive control of microgrid dual active bridge converters connected to battery storage [52]. Despite being mostly limited to single devices or strictly bounded subsystems, these studies lay the methodological foundation for more advanced AI-driven integration by establishing feature engineering, supervised learning, and local optimisation [53-55].

The system boundary is moved to the facility level by the second evolutionary layer in Table 4 and Fig. 4, which aggregates AI from devices into complete assets like buildings, car fleets, and processing plants. This trend is exemplified by the use of explainable artificial intelligence in data-driven estimation of building energy consumption and related greenhouse gas emissions, which converts high-dimensional building data into interpretable indicators that aid in the design of policies and renovation strategies [56]. In order to transform EV fleets into manageable demand and storage assets, temporal charge profiling of electric vehicles reveals usage patterns that guide infrastructure sizing, load management, and smart-charging algorithms [57]. At the water-energy nexus, hybrid desalination technologies demonstrate how AI-enabled process design can synchronise membrane, electrical, and thermal subsystems for a more sustainable freshwater supply [58]. Asset-level innovations in photovoltaic systems continue this trend: UAV-enabled fault detection using rough set theory increases reliability and inspection effectiveness in large-scale PV fields [59], while numerical

modelling and neural-network-based optimisation of advanced solar panels increases conversion performance [60]. As in smart-tropical building control, building-focused digital twins and deep learning architectures for customised thermal comfort indicate a developing ability to combine occupant-centric goals with energy efficiency at the single-building scale [4]. By integrating forecasting, control, and optimisation into buildings, plants, and fleets, these studies collectively transform artificial intelligence (AI) from a device-centric tool to a facility-scale intelligence layer [61].

Several sectors and vectors are co-optimized under techno-economic and environmental goals in the third stage, which is marked by a clear shift towards system-centric AI-driven integrated energy systems (Table 4 and Fig. 4). The techno-economic evaluation of coordinated energy management in multi-vector systems with subterranean storage and AI-assisted maritime scheduling, which integrates gas, electricity, and logistics into a single corridor rather than treating them as separate infrastructures, serves as evidence of this development [2]. Probabilistic energy management in hydrogen-integrated microgrids with vehicle-to-grid capabilities serves as an example of how AI frameworks can coordinate renewables, storage, hydrogen, and mobility within a single operational envelope [18]. Biomass-driven solid oxide fuel cell plants that simultaneously produce electricity and ammonia and optimise them using machine-learning-assisted tri-objective frameworks extend integration to the power-fuel-chemical nexus [62]. AI-driven biogas production optimisation at water resource recovery facilities, where energy circularity and carbon neutrality targets are jointly addressed, makes water–energy–waste synergies clear [17]. Hybrid district heating and heat pump portfolios also exhibit system-level integration, as modelling of hybrid energy systems captures the interplay between electricity supply and heat networks [63]. The technological and control issues that arise when heterogeneous resources are integrated into robust hybrid renewable energy systems are documented in complementary reviews of hydrogen, biomass, biogas, and PV hybrid systems [64]. Digital twin frameworks for microgrids and building stocks begin to offer high-fidelity virtual testbeds for complex integrated systems' planning, stress testing, and lifecycle management during this phase [65].

An ecosystem-centric, AI-native paradigm is projected in the last stage shown in Table 4 and Figure 4, where communication networks, computation platforms, and energy infrastructures are all co-designed as a single cyber-physical fabric. By integrating learning and control into the very framework of next-generation communication systems, sustainable 6G architectures view energy efficiency and AI-native design principles as fundamental rather than auxiliary [66]. Future grids will operate as joint energy–information systems, where resource allocation spans both power flows and data pathways, according to surveys of integrated sensing, communication, and computation [19]. By enabling distributed learning and control across vast areas and multi-layer infrastructures, federated LoRaWAN architectures for far-edge IoT and service-oriented space–air–ground integrated networks with pervasive intelligence expand the geographical and topological scope of artificial intelligence (AI) [67, 68]. Applications in agriculture and urban areas demonstrate the socio-ecological depth of this evolution: While intrusion-detection schemes and critical-infrastructure vulnerability analyses indicate the growing importance of cybersecurity as an intrinsic dimension of AI-driven energy ecosystems, AI–blockchain frameworks for secure smart grids and smart building management [69, 70] imply new market and trust architectures at the governance and security frontier. When combined, these contributions show that AI-driven integrated energy systems are moving towards multi-layered, AI-native ecosystems where the

institutional, digital, and physical layers are intertwined. Table 4 provides a structured lens through which to view this shift [71-74].

**Table 4.** Evolutionary stages of AI-Driven Integrated Energy Systems

| Stage ID  | Conceptual label                                                            | Approximate temporal focus in corpus                                                                              | Dominant AI role & methods                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        | System boundary & integration scope                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |
|-----------|-----------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Stage I   | Component- and device-centric AI augmentation                               | 2019–early 2020s, foundational work extended by recent device optimisation studies                                | AI mainly augments single components through supervised learning, neural networks and pattern recognition; models act as fast surrogates for complex physics or control surfaces, often trained on experimental or simulated data (e.g., neural-network-based optimisation of adsorption chillers and thermodynamic subsystems, [49]). Early structural health monitoring uses machine learning for pattern recognition on self-powered sensing signals [50], while prognostics and health management employs data-driven degradation models for hybrid marine energy systems [51]. Later contributions extend this logic to advanced materials and devices, such as MXene-based solar fluids optimised via AI [46] and nanostructured neuromorphic devices characterised with smart conductance modelling [200]. | System boundary is local and component-level: individual PV modules, chillers, power-electronics interfaces, structural elements, batteries, or novel energy materials. Integration is primarily vertical (device ↔ controller ↔ local sensor) rather than horizontal across vectors or sectors. Adaptive control of dual active bridge converters in microgrid battery systems typifies power-interface-focused intelligence [52]. Numerical modelling and neural-network optimisation for advanced PV efficiency remain confined to the module or string scale [60].                                                        |
| Stage II  | Asset-level intelligent energy systems (buildings, plants, fleets)          | 2020–2024, with strong growth from 2022 onward                                                                    | AI shifts to full assets (buildings, EV fleets, desalination plants, microgrids) using deep learning, explainable AI, and GANs. Building energy and GHG estimation exploits explainable ML models that infer consumption patterns from rich feature sets [56]. Digital twin-based and deep-learning frameworks deliver personalised thermal comfort and energy-efficient HVAC control in smart buildings [4]. In mobility, data-driven temporal charge profiling reveals EV usage trajectories for asset-aware charging strategies [57], while bio-inspired AI optimises regenerative braking in bus fleets to improve energy recovery [91]. Process industries deploy ML-accelerated design for fractured geothermal systems [179] and GAN-enhanced robust optimisation for PV grid integration [23].            | System boundary expands to single sites or asset clusters: individual buildings or campuses, specific EV fleets, desalination or geothermal plants, or single microgrids. Integration occurs among subsystems (thermal, electrical, comfort, process units) within a defined facility. Smart-building frameworks manage HVAC, storage and envelope operation under local constraints [86]. PV cooling and dust mitigation solutions use IoT-connected intelligent controllers at plant level [201]. Role-of-redox-flow-battery and AI controllers in weak microgrids marks an asset-level view of storage-grid coupling [77]. |
| Stage III | System-level multi-vector, multi-sector AI-Driven Integrated Energy Systems | 2023–2025, consolidating around integrated hydrogen, multi-carrier microgrids and WEF (water–energy–food) nexuses | AI becomes the coordination engine for interacting carriers and sectors. Techno-economic assessment of multi-vector systems with underground storage and AI-based maritime scheduling links electricity, gas and logistics in coordinated planning [2]. Hydrogen-integrated microgrids using probabilistic AI-driven hybrid control and vehicle-to-grid form a unified framework for power, hydrogen and mobility [18]. Biomass-driven SOFC plants co-producing electricity and ammonia, optimised via ML-assisted tri-objective frameworks, exemplify power–fuel–chemical integration [62]. AI-enhanced frameworks for biogas production in water resource recovery facilities strengthen the circularity of water–waste–energy cycles                                                                           | System boundary is regional or network-level, spanning multi-carrier microgrids, district heating networks, integrated industrial sites, or city-scale WEF systems. Hybrid energy systems with heat pumps and district heating reflect coordinated operation of thermal and electrical networks [63]. Hydrogen refuelling stations sized via AI-based optimisation of hybrid supply demonstrate corridor-level integration between generation, storage and transport demand [3]. Mega-scale decarbonised industrial parks using generative AI for techno-economic and environmental                                           |

|          |                                                                     |                                                 |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
|----------|---------------------------------------------------------------------|-------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
|          |                                                                     |                                                 | [17]. Systematic reviews of hybrid renewable energy systems map configurations that couple hydrogen, biomass, biogas and PV across multiple vectors and load types [64].                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | assessment suggest campus-scale coordination across process units, utilities and renewables [24].                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |
| Stage IV | Ecosystem-scale, AI-native energy–information–mobility–urban system | 2024–2025 frontier, projecting toward 2030–2050 | AI is embedded as a native layer in coupled energy–information infrastructures, leveraging generative AI, federated learning, multi-agent DRL and edge intelligence. Sustainable 6G architectures explicitly co-design communication and energy efficiency, treating AI-native networking as the backbone for future integrated systems [66]. Surveys on integrated sensing, communication and computation describe platforms where data, control and energy services are jointly optimized [19]. Federated LoRaWAN architectures and service-oriented space–air–ground integrated networks with pervasive intelligence enable far-edge and multi-layer coordination of IoT devices and grid assets [68, 67]. Generative spatial AI for smart cities uses large-flow models to align urban form, mobility and energy flows with sustainability objectives [89], while AI-augmented smart irrigation systems powered by solar PV and IoT unify water, food and energy resilience [122]. | System boundary expands to urban, regional or even planetary ecosystems, where energy systems co-evolve with communication, transport, water, food and digital infrastructures. Digital twins operate at building-stock and microgrid levels for renovation roadmaps and health management of distributed assets [87, 65]. AI–blockchain frameworks in smart grids embed trust and transaction logic directly into the cyber-physical infrastructure [69]. Security and vulnerability assessments capture systemic risk arising from large-scale AI integration in critical infrastructure [70] and fire hazard detection in solar plants through UAV–SCADA–AI ensembles [141]. |

## 5. Classification of AI–Driven Integrated Energy Systems

### 5.1 System-Scope Classification by Energy Vectors, Configuration, and Spatio-Temporal Scale

The 153-reference corpus is arranged along three orthogonal axes (energy vectors, configuration topology, and spatio-temporal scale) in Table 5 and Fig. 5, which show how AI gradually reorganises integrated energy systems from local, mono-vector assets to intricate, multi-sector ecosystems. Early contributions focus on power-electronic subsystems and electricity-only devices, combining AI for control, prognostics, and efficiency optimisation in separate components like PV modules, converters, and adsorption chillers [49]. This reasoning is expanded in later research from individual assets to buildings, microgrids, and industrial facilities, where AI manages several subsystems inside a common site perimeter [56]. More recent research shifts to fully integrated multi-vector configurations, often framed within power-to-X, water-energy-waste, or city-scale smart-infrastructure narratives, that couple electrical, hydrogen, thermal, and chemical carriers [64]. The temporal horizons of device-scale control at millisecond-to-minute resolution, asset operation over hours-to-days, and multi-decade planning for decarbonisation and resilience are all closely related to energy vectors and configurations across the Table 5 [1, 75].

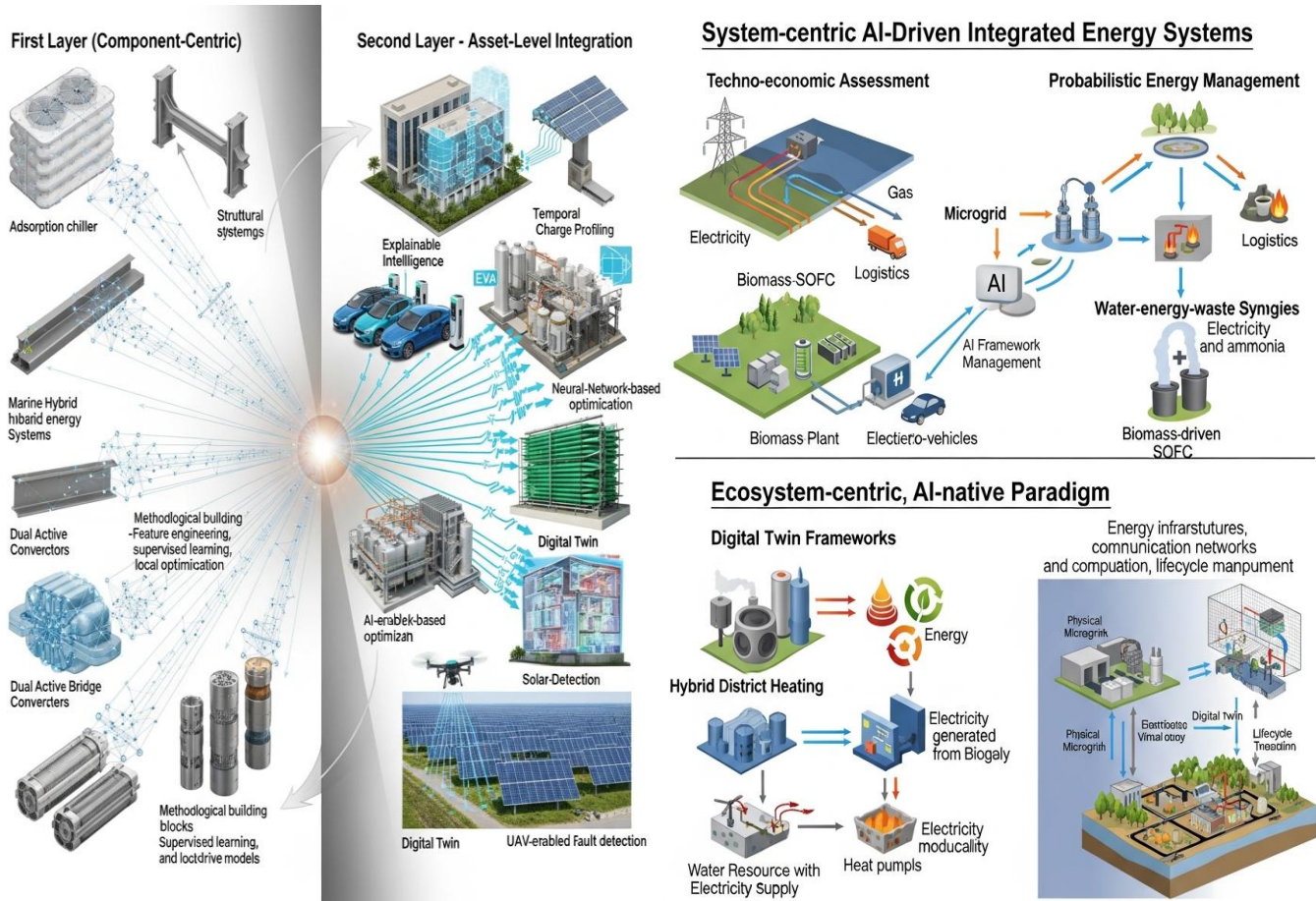


**Fig. 4.** Evolutionary stages of AI-Driven Integrated Energy Systems

**Table 5.** System-scope classification by energy vectors, configuration, and spatio-temporal scale

| System-scope tier                 | Dominant energy vectors represented in the corpus                                                                                                      | Typical system configurations                                                                                       | Spatial scale                    | Dominant temporal focus in the corpus                                                               | Approx. no. of studies (n) | Representative examples*                                                                                                                                                                                                            |
|-----------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------|----------------------------------|-----------------------------------------------------------------------------------------------------|----------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 1. Device / component / converter | Mainly electricity (power electronics, PV modules, batteries, fuel cells); isolated instances of H <sub>2</sub> /Power-to-X and water/thermal coupling | PEMFC/SOFC stacks, PV modules, battery cells/management, nanoscale harvesters, inverters, electro-thermal materials | Device / component scale         | Mostly unspecified or multi-horizon, with subsets on real-time behaviour and lifetime / degradation | 23                         | Ayadi et al. [45] – AI-enhanced PEMFC performance; Mamodiya et al. [60] – NN optimisation of solar panel efficiency; Ozkan & Ozkan [121] – neural-network battery management; Jiang et al. [202] – AI-based PEMFC flow-field design |
| 2. Asset / building / facility    | Electricity + heat/cooling dominate (BIPV,                                                                                                             | Individual buildings (residential,                                                                                  | Single-building / facility scale | Mixed: operational control and                                                                      | 20                         | Heydari et al. [203] – AI-assisted two-                                                                                                                                                                                             |

|                                             |                                                                                                                                                   |                                                                                                                                   |                                   |                                                                                                                      |    |                                                                                                                                                                                                                                                                                                                          |
|---------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------|-----------------------------------|----------------------------------------------------------------------------------------------------------------------|----|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
|                                             | HVAC, data-centre cooling); some integration with water and H <sub>2</sub>                                                                        | commercial, schools), data centres, manufacturing facilities, wastewater/energy plants                                            |                                   | hourly–daily forecasting, plus planning / retrofit analysis                                                          |    | phase data centre cooling; Elaziz Waseef [169] – BIPV integration review; Almadhor et al. [4] – digital-twin residential energy modelling and smart-building comfort control; Kim et al. [86] – AI-optimised control for carbon-neutral buildings                                                                        |
| 3. Local multi-energy hub / microgrid       | Predominantly electricity coupled with storage; a subset includes H <sub>2</sub> /Power-to-X and gas/biogas, occasionally linked to mobility      | Islandable microgrids, hybrid PV–wind–battery–fuel-cell systems, hydrogen-integrated microgrids, micro gas-turbine hubs           | Campus / estate / community scale | Strongly operational (minute–hour dispatch, frequency regulation), with some multi-year techno-economic design       | 7  | Khosravi et al. [18] – AI-driven hybrid control in hydrogen microgrids; Pajooh et al. [77] – AI-based control with redox flow batteries in weak microgrids; Banihabib et al. [160] – AI-optimised micro gas turbine in NG/H <sub>2</sub> microgrids; Ebrahimi et al. [65] – digital-twin health management in microgrids |
| 4. Urban district / city / smart city       | Coupled electricity–mobility, with additional heat/cooling and renewables integration; beginning to include UAV logistics and urban digital twins | District-scale energy and mobility systems, smart-city mobility infrastructures, UAV-assisted logistics, city-level digital twins | District / city scale             | Combination of real-time / near real-time operations (e.g., bus energy management) and scenario-based urban planning | 10 | Ekici et al. [91] – bio-inspired AI for electric bus energy efficiency; Reis et al. [94] – IoT architecture for low-emission smart-city mobility; Huang et al. [89] – generative spatial AI for smart-city digital twins; El-Barbary et al. [96] – AI + IoT for wind in smart cities                                     |
| 5. Industrial park / sector-coupled cluster | Multi-vector: electricity, heat, fuels, H <sub>2</sub> , and process streams; strong process–energy coupling                                      | Petrochemical parks, mining sites, integrated industrial parks, water resource recovery facilities                                | Cluster / industrial-park scale   | Primarily techno-economic and environmental planning over multi-year horizons, with some operational optimisation    | 2  | Heo et al. [24] – generative-AI-driven decarbonised industrial park in petrochemicals; Patil et al. [204] – AI to reduce environmental impact in the mining sector                                                                                                                                                       |

|                                               |                                                                                                                                                                                                         |                                                                                                                                                       |                                                                                                             |                                                                                                                         |    |                                                                                                                                                                                                                                                                                                                               |
|-----------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------|----|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 6. Regional / national / infrastructure       | System-level electricity often co-evolving with mobility/transport, H <sub>2</sub> and occasionally heat                                                                                                | Smart grids, PV–FC grids, integrated EV charging networks, 5G/6G-enabled smart energy infrastructures, national-scale hydrogen value-chain/EV systems | Regional / national scale                                                                                   | Mix of operational scheduling (e.g., EV charging, grid-tied hybrids) and multi-year techno-economic / policy assessment | 18 | Nene & Thankachan [15] – AI-based optimisation of grid-tied PV–fuel-cell hybrids; Taghizad-Tavana et al. [92] – H <sub>2</sub> production to AI energy management in H <sub>2</sub> FCEVs; Oukhouya & Jamila [181] – PV–BESS EV charging stations; Salman [102] – AI-driven energy security under Russian gas exit            |
| 7. Cross-cutting digital / AI / enabling tech | Indirectly spans all vectors; often abstracted from specific carriers but directly relevant to AI–IES (e.g., smart grid intrusion detection, federated learning, edge AI, 6G networks, AI accelerators) | ICT backbones, edge/cloud platforms, AI accelerators, digital-twin middleware, cyber-security frameworks, 6G/O-RAN, SAGIN networks                    | Cross-scale: from chip and device level through edge nodes to global communication and cloud infrastructure | Broad spectrum: real-time inference, operational management, and strategic outlook / survey                             | 73 | Safari et al. [1] – AI in power electronics; Abou-Elasaad et al. [98] – smart-grid intrusion detection; Akgül et al. [66] – sustainable 6G architecture; Wu et al. [19] – AI-enabled integrated sensing, communication and computation survey; Ebrahimi et al. [65] – DT-driven microgrid health management (ICT perspective) |

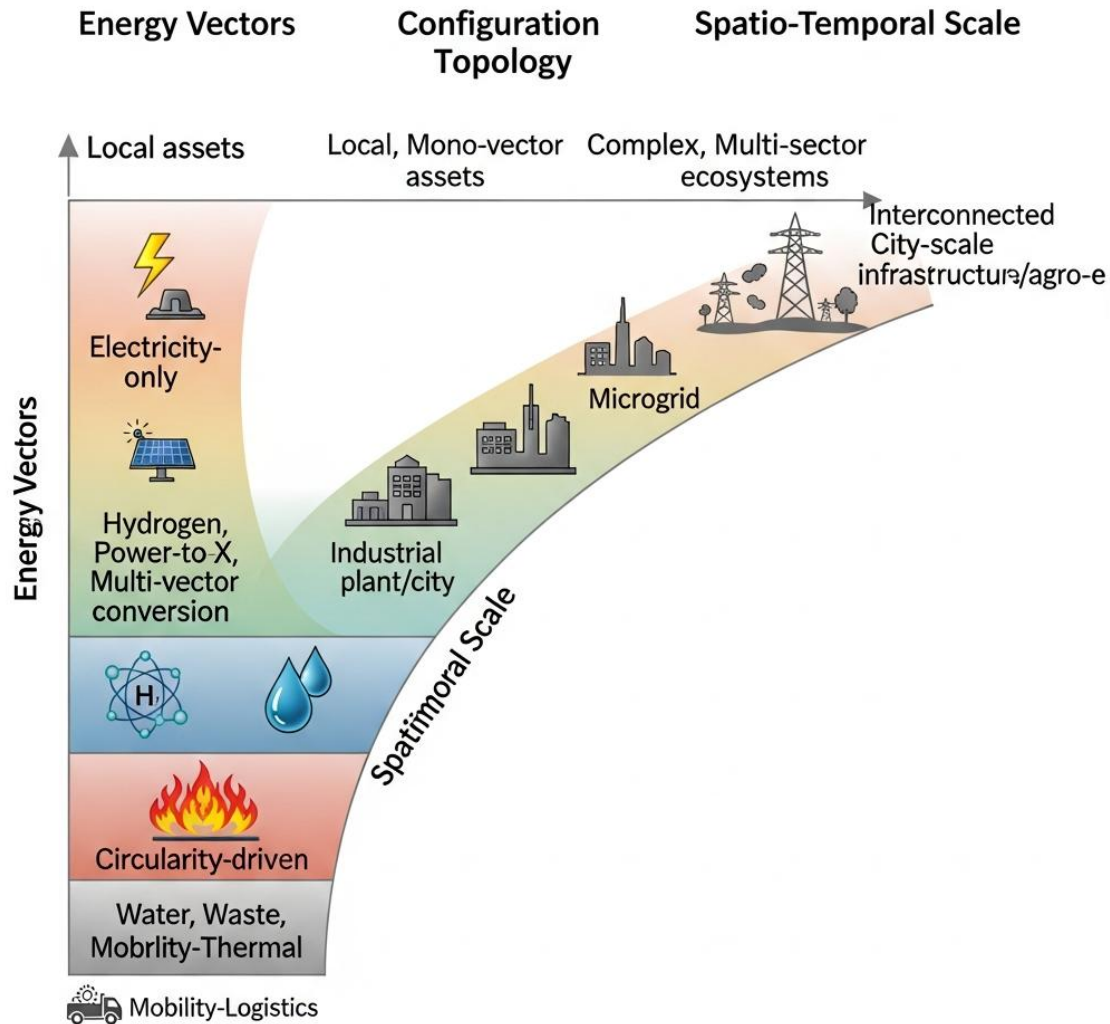


**Fig. 5.** System-scope classification by energy vectors, configuration, and spatio-temporal scale

### 5.1.1 Electricity-Centric Systems

Table 5 and Figure 6's first block classifies electricity-centric systems, such as PV plants, microgrids, and geothermal installations, where AI primarily affects single or coupled electrical vectors but operates within physically defined boundaries. PV-focused works on automated PV power prediction, AI-driven solar trackers, and GAN-enhanced robust optimisation for grid integration [76] illustrate this mono-vector but increasingly high-dimensional space of electrical assets. AI-based controllers for redox-flow batteries, micro gas turbines, and dual active bridge converters are used in microgrid-focused research, integrating intelligent optimisation into distribution-scale local power networks [77]. These configurations align AI's predictive and control capabilities with power-quality management, frequency regulation, and short-term scheduling, and they typically operate on operational horizons ranging from seconds to days [78]. From feeders and feeder endpoints to campus-scale microgrids, the table illustrates how these systems, which are still primarily single-vector in terms of energy, already require non-trivial spatial granularity.

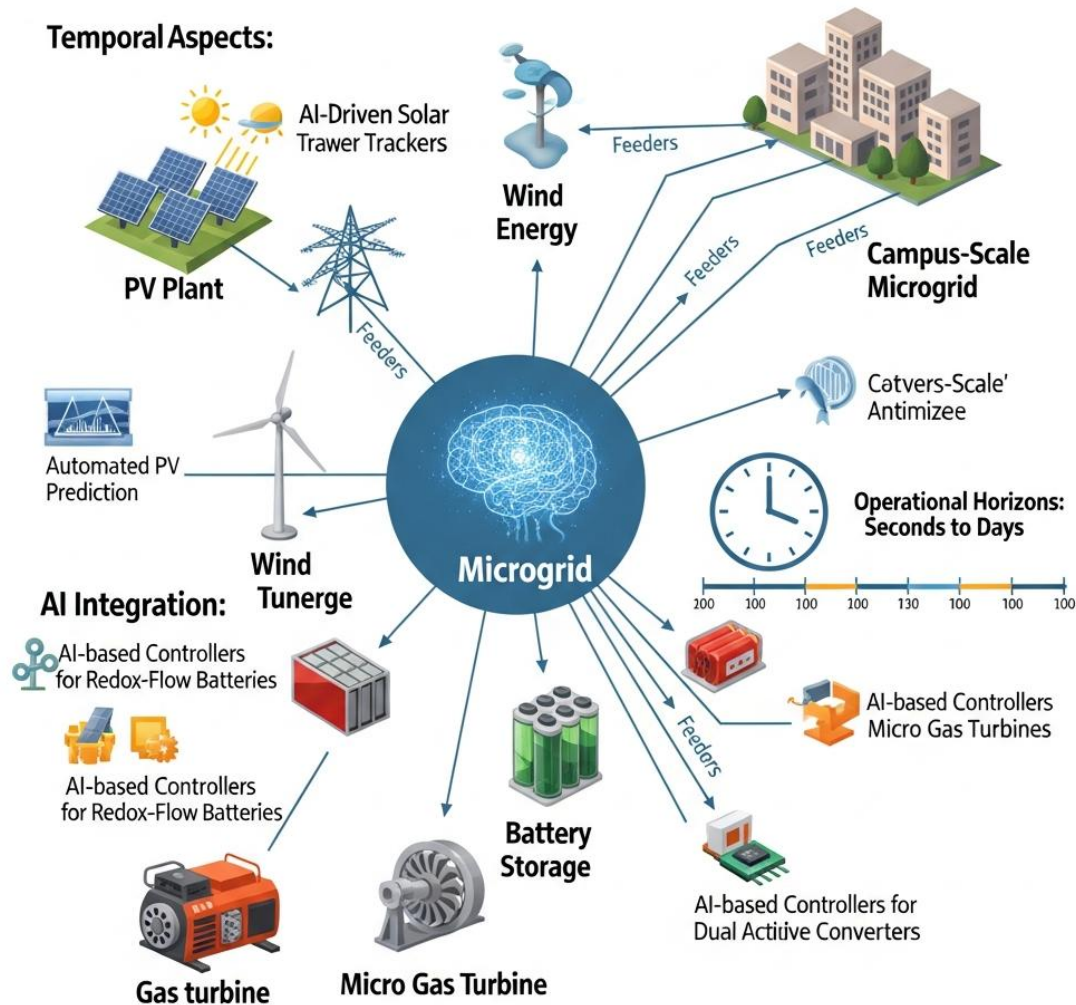


**Fig. 6.** System-scope classification of AI-Driven Integrated Energy Systems utilizing Electricity-centric systems

### 5.1.2 Hydrogen, Power-to-X, and Multi-vector Conversion Chains

AI coordinates flows across electricity, hydrogen, fuels, and chemical products at both plant and regional scales in a second cluster in Table 5 and Fig. 7, which covers hydrogen, power-to-X, and multi-vector conversion chains. The technological-economic optimisation of integrated gasification fuel cells with carbon capture, biomass-driven SOFC-ammonia plants, and green dimethyl ether production [79]; Dou et al. [62]; Zamora-Aguirre et al. [80]) demonstrate how electricity, heat, hydrogen, and value-added chemicals form tightly coupled conversion networks. Hydrogen refuelling station design and hydrogen-integrated microgrids, frequently with vehicle-to-grid interfaces, introduce vector links between centralised or distributed generation, storage, and transport demand [18]. Reviews of AI in hydrogen systems and hydrogen-battery technologies highlight sector coupling beyond single sites, expanding this picture across global supply chain, mobility, and storage contexts [81, 48]. Table 6 associates multi-vector configurations with long-term timescales in these entries: planning horizons of years, project lifetimes of decades, and operational choices ranging from seasonal storage management to minute-level dispatch.

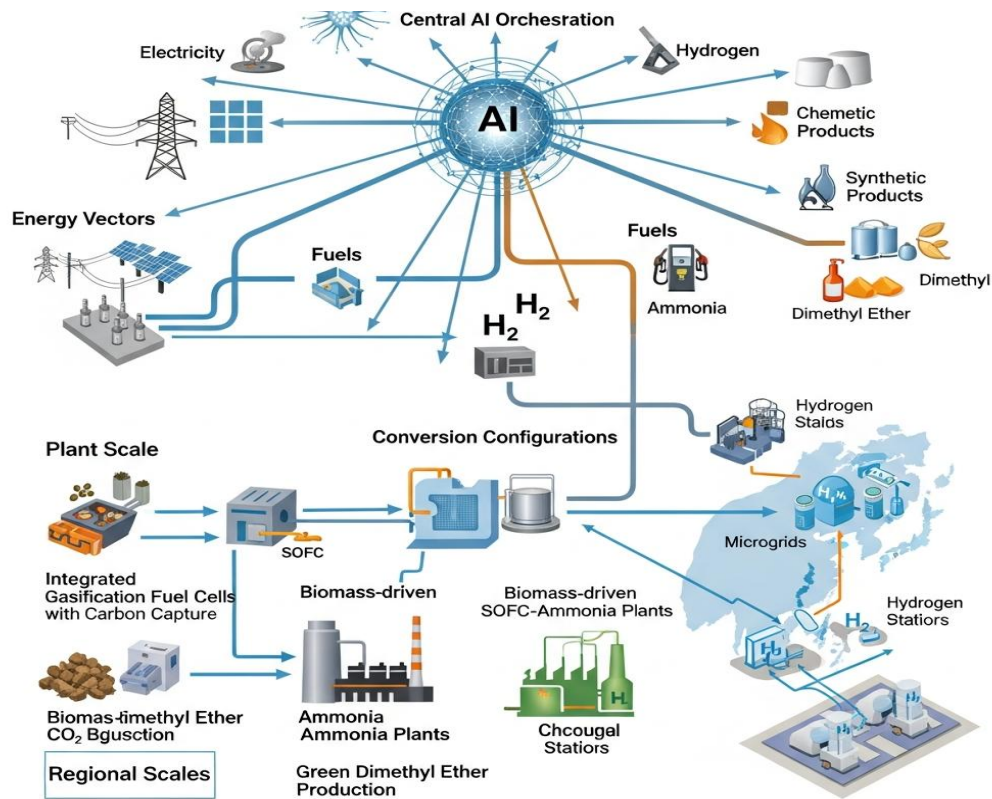


**Fig. 7.** System-scope classification of AI-Driven Integrated Energy Systems utilizing hydrogen, power-to-X, and multi-vector conversion chains

### 5.1.3 Water-, Waste- and Circularity-Driven Energy Systems

Table 5 and Fig. 8 further isolates water-, waste- and circularity-driven energy systems as a distinct system-scope archetype, where AI coordinates bio-physical flows instead of purely electrical quantities. With plant-scale assets integrated into city-scale sanitation and energy planning, AI-optimized biogas production in water resource recovery facilities demonstrates circular integration between wastewater treatment, energy recovery, and greenhouse gas mitigation [17]. In the water sector, net-zero strategies frame water utilities as energy prosumers in larger multi-vector networks, connecting regional decarbonisation pathways with local operational optimisation [82]. The performance of microalgae-based wastewater-to-bioenergy systems is dependent on catchment-scale boundary conditions as well as facility configuration. These systems treat biomass, nutrients, electricity, and heat as a coupled resource system [83]. Hybrid desalination, which uses renewable energy sources and AI-enabled process optimisation, is an example of a water-energy nexus where spatiotemporal scales range from membrane module dynamics to coastal resource planning [58, 84]. Table 6 in this block highlights how AI supports long-term circular resource management across basins and urban areas, as well as intra-plant coordination.

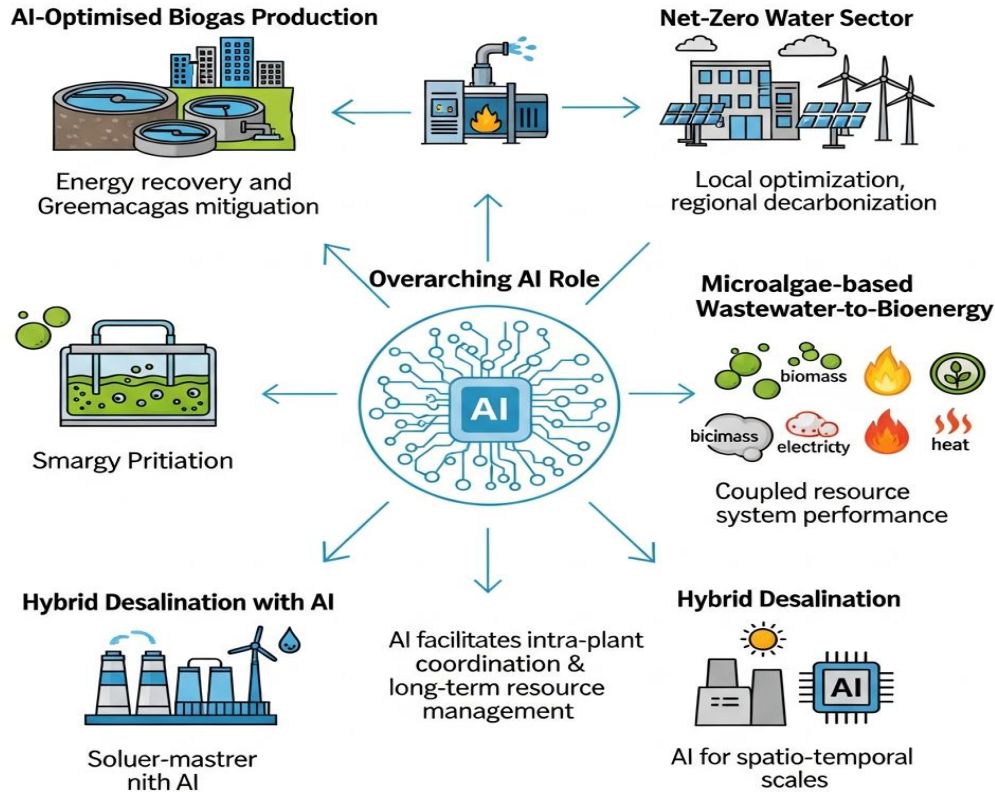


**Fig. 8.** System-scope classification of AI-Driven Integrated Energy Systems utilizing waste- and circularity-driven energy systems

#### 5.1.4 Building-, District- and City-scale Electricity–Thermal Systems

Building-, district-, and city-scale electricity-thermal systems are the subject of another significant category. In these systems, energy vectors comprise not only electricity but also heat, cooling, and frequently embodied carbon flows. Deep learning frameworks for customised thermal comfort and digital twin-enabled residential energy models demonstrate asset-level and room-level configurations where AI synchronises HVAC operation with building envelopes and occupant needs [85]. Ontology-enabled AI agents for building operation and maintenance extend this logic to asset portfolios, allowing for multi-building optimisation and life-cycle asset management within campus or district boundaries [86]. Fuzzy decision-support systems for nature-based retrofits and city-scale morphological classification of school building stocks place building-level interventions within urban renovation roadmaps, emphasising spatial aggregation from individual buildings to stock-level clusters [87, 88]. Generative spatial AI for sustainable smart cities pushes the system boundary to entire urban regions where long-term planning scenarios jointly explore energy use, land-use patterns, and mobility flows [89]. Sub-hourly set-point control, multi-decadal renovation cycles, and infrastructure lock-in dynamics are among the temporal scales shown in this section of Table 5 and Fig. 9.

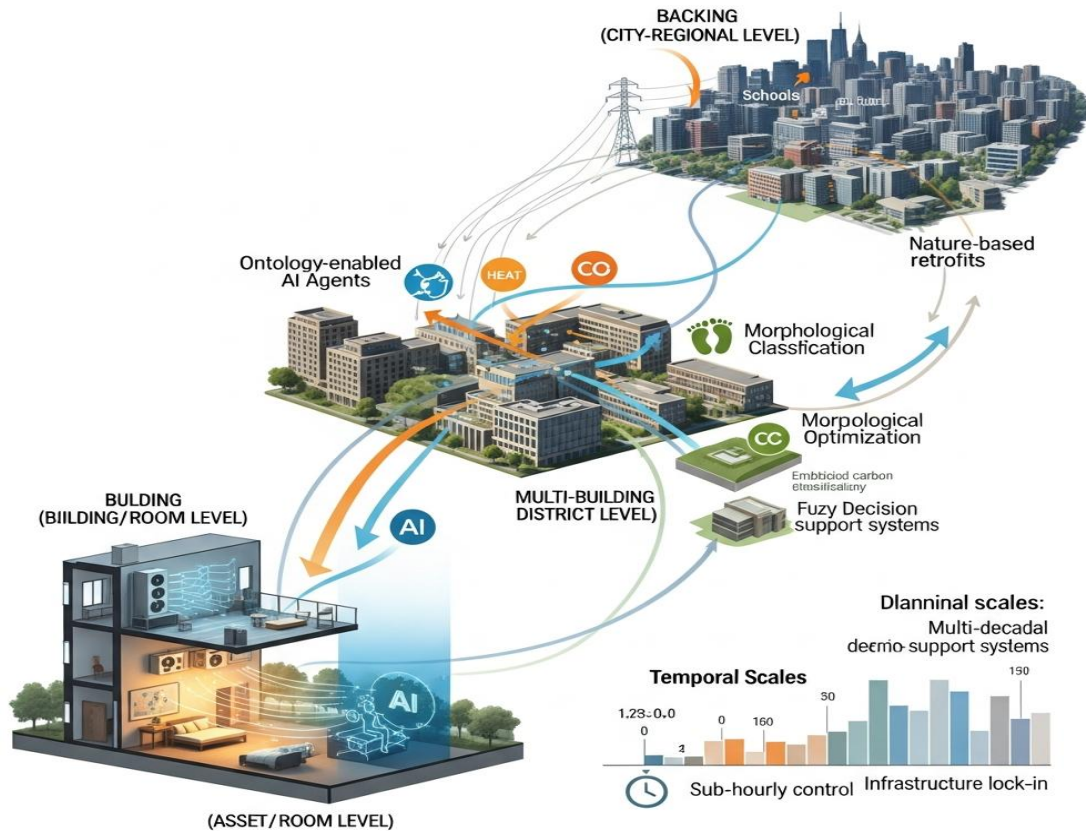


**Fig. 9.** System-scope classification of AI-Driven Integrated Energy Systems utilizing building-, district- and city-scale electricity-thermal systems

#### 5.1.5 Mobility- and Logistics-Oriented Entries

Another system-scope archetype is formed by mobility- and logistics-oriented entries in Table 5 and Fig. 10, where energy vectors interact with spatiotemporal patterns of movement across airspace, roads, and maritime corridors. At hourly-to-daily temporal resolutions, data-driven temporal charge profiling for EVs matches charging demand with network constraints across corridor and urban scales [57]. This is further extended into multi-vector coupling, where local generation and storage dynamically interact with fleet charging profiles by AI-driven optimisation frameworks for smart EV charging systems integrated with PV and battery storage [90]. Real-world regenerative braking optimisation in electric buses shows AI operating at vehicle-dynamics temporal scales while still respecting route-level energy constraints [91]. By connecting individual vehicles to the grid, hydrogen infrastructure, and communication networks, hydrogen fuel cell electric vehicles and V2X modes of operation expand configurations to regional transportation and distribution networks [92]. AI coordinates energy, logistics, and storage decisions across days and seasons in maritime scheduling, which extends this logic into port-to-port trade and shipping corridors in multi-vector systems [2]. Thus, mobility systems with extremely irregular spatiotemporal scales—from millisecond-level control to seasonal fleet planning—are linked in Table 6.

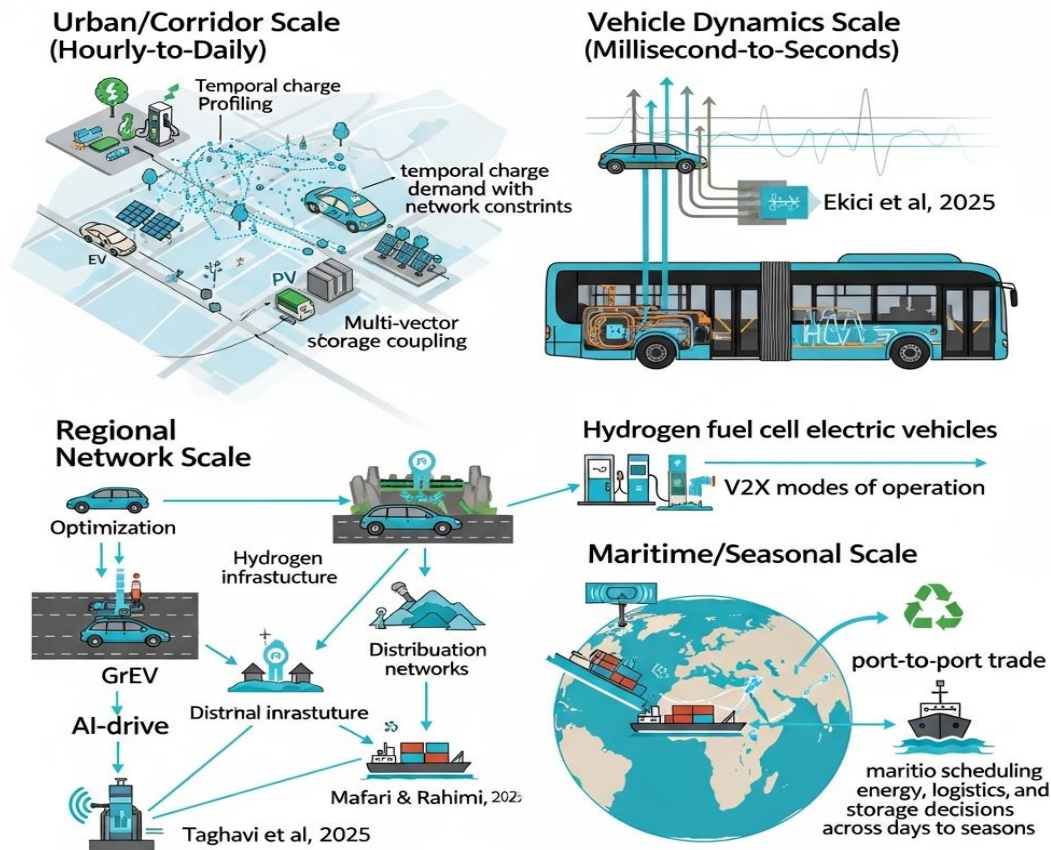


**Fig. 10.** System-scope classification of AI-Driven Integrated Energy Systems utilizing Mobility- and logistics-oriented entries

#### 5.1.6 Ecosystem-scale smart-city and agro-ecosystem configurations

Ecosystem-scale Smart-city and agro-ecosystem configurations, where energy vectors intersect with water, food, and environmental services across large territories, are also highlighted in Table 5 and Fig. 11. Solar PV-powered AI-enhanced smart irrigation systems demonstrate direct water-energy-food coupling at the field level, but they have obvious ramifications for basin-level water security and rural energy access [85, 93]. IoT-based architectures for sustainable urban mobility, AI-enhanced UAVs for urban logistics, and AI-driven IoT frameworks for wind monitoring are examples of this convergence of mobility, logistics, and energy in urban air and ground spaces [94, 95, 96]. When combined with federated edge architectures, digital twin-driven health management in microgrids can be extended to urban distribution networks, allowing geographically scattered assets to function as coordinated energy ecosystems [65, 68]. Energy and information infrastructures are presented as co-designed layers of future urban systems by integrated sensing, communication, and computation surveys and sustainable 6G architectures. This pushes the system scope towards planetary-scale networks with nested local subsystems [97]. This category includes temporal scales ranging from near-real-time sensing and action to long-term planning horizons for cities that are climate-neutral and climate-resilient.

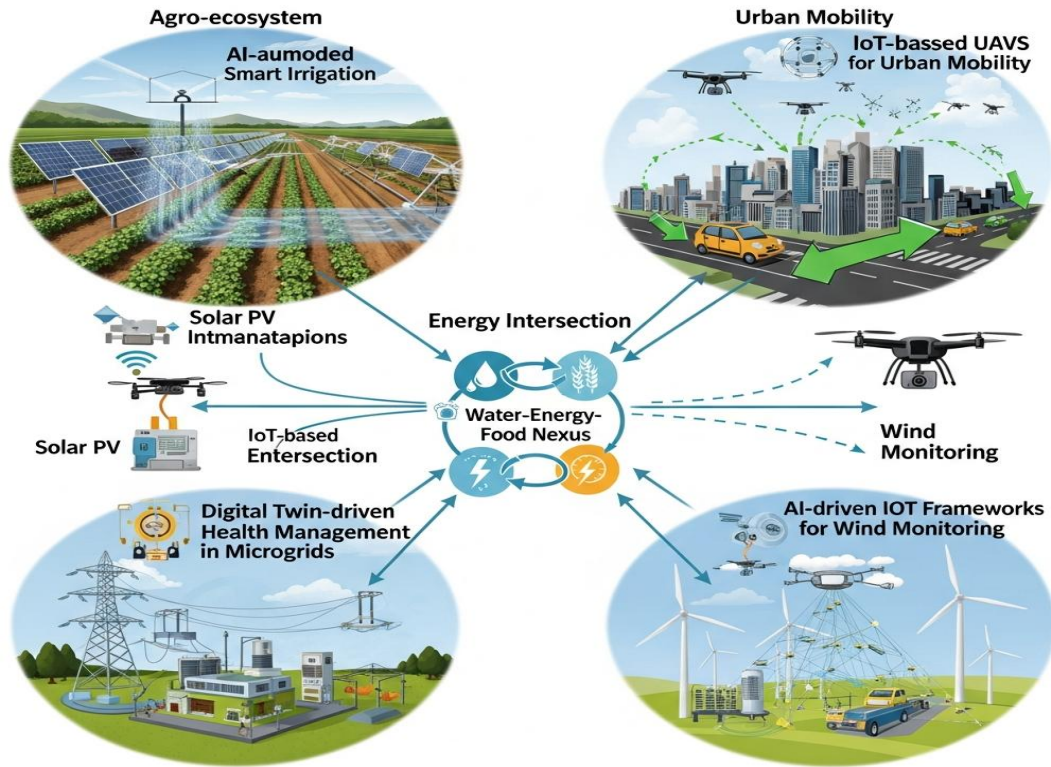


**Fig. 11.** System-scope classification of AI-Driven Integrated Energy Systems utilizing ecosystem-scale smart-city and agro-ecosystem configurations

#### 5.1.7 Cyber-Physical and Governance-Oriented Systems

Last but not least, Table 5 and Fig. 12 outline a cross-cutting class of cyber-physical and governance-oriented systems, in which energy carriers coexist with information, trust, and risk as the dominant "vector". Grid configurations where cyber-security is a core component of system design rather than an afterthought are encapsulated in AI- and blockchain-based frameworks for secure smart-grid and power distribution automation [69]. Under near-real-time constraints, AI-driven intrusion detection for smart grids and critical infrastructure studies emphasise a system scope that extends from substation-level protection to national and transnational infrastructure networks [98, 70]. Knowledge-centric VLSI systems, cloud-based AI labs, and sustainable hiring practices demonstrate how AI energy-system intelligence is dependent on digital labour architectures and underlying compute fabrics, which are both energy-intensive and dispersed geographically [99, 100, 101]. Mega-scale decarbonized industrial parks and national energy-security plans during gas supply crises highlight policy-driven system boundaries that function across national grids, industrial clusters, and geopolitical timeframes [24, 102]. Table 6 demonstrates that, rather than merely engineering control intervals, AI-driven integrated energy systems are increasingly occupying a governance landscape where spatiotemporal scales correspond with regulatory cycles, investment lifetimes, and systemic risk horizons.

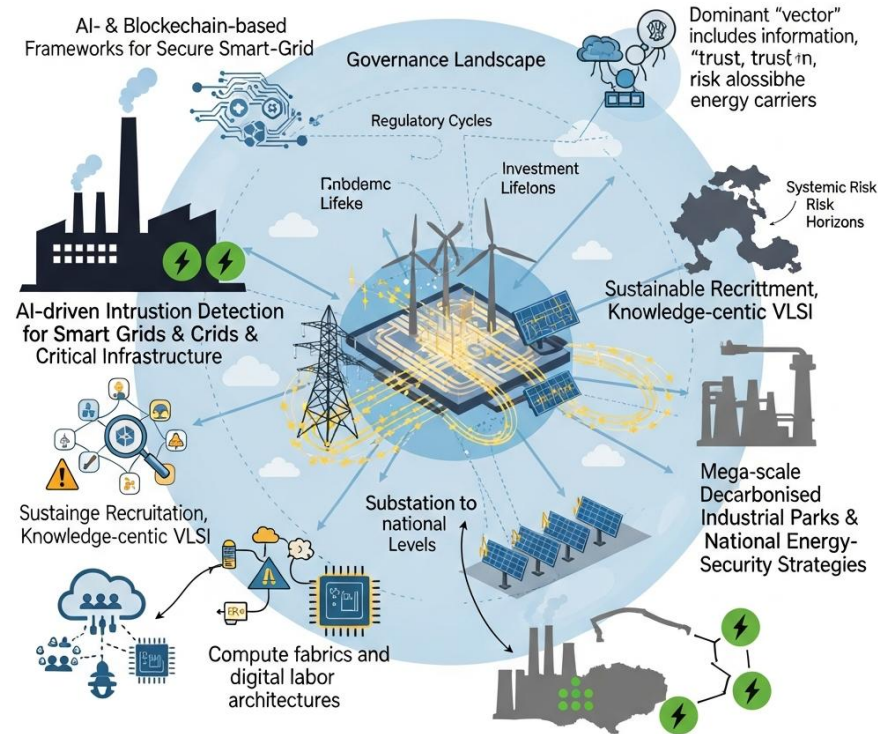


**Fig. 12.** System-scope classification of AI-Driven Integrated Energy Systems utilizing cyber-physical and governance-oriented systems

## 5.2 AI-Methods Classification by Data and Deployment Architecture

A system-level view of how AI is actually integrated into integrated energy systems is provided by Table 6 and Fig. 13, which group the 153-paper corpus into eight AI-method clusters that differ not only by algorithms but also by data regimes and deployment architectures. While hardware-oriented accelerators and 6G/LoRaWAN architectures anchor a shift towards pervasive edge and federated intelligence, supervised deep learning clusters at one extreme centre on large, SCADA-scale time series for forecasting and control. Based on reviews of next-generation power electronics and AI applications across energy domains, this multi-axis classification shows that integrated energy systems are no longer solely algorithm-centric but are increasingly shaped by opportunities and constraints in data acquisition pipelines, communication infrastructure, and on-device compute [97]. Therefore, the table serves as a link between actual deployment patterns across buildings, grids, transportation, water, and industrial energy systems and methodological taxonomies [103].

**Table 6.** AI-methods classification by data and deployment architecture

| Cluster ID                                                             | Dominant AI methods & typical algorithms in Table 1                      | Typical training data sources & indicative scale                                                                                                  | Dominant deployment architecture                                                                       | Evidence density | Representative topics / examples*                                                                                                                                                                             |
|------------------------------------------------------------------------|--------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------|------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| AM-1: Supervised deep learning for time-series and tabular forecasting | LSTM/GRU, temporal CNNs, transformers, hybrid RNN-LSTM, deep feedforward | Operational time series from grids, buildings, EV fleets, PV plants, heat networks; usually field SCADA/IoT datasets with $10^4$ – $10^6$ samples | Mostly centralised/cloud EMS or forecasting servers, occasionally cloud-integrated (e.g., virtual EMS) | High             | Stacked temporal deep learning for degradation of Li-metal batteries; LSTM-driven solar forecasting and residential energy management; regional heat-load forecasting with adversarial training; power-demand |

|                                                                                      |                                                                                                                                                                     |                                                                                                                                                                                                                      |                                                                                                                                                                |                                |                                                                                                                                                                                                                                                                                                                                                                                                                                                     |
|--------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
|                                                                                      | networks for regression                                                                                                                                             |                                                                                                                                                                                                                      |                                                                                                                                                                |                                | forecasting with multimodal feature discovery; emission forecasting in automotive systems; day-ahead load forecasting for power systems.                                                                                                                                                                                                                                                                                                            |
| AM-2: Spatial / vision / generative deep models                                      | CNNs, encoder–decoder architectures, GANs (standard and knowledge-integrated), generative spatial AI and AutoML frameworks                                          | UAV imagery over PV fields, satellite/remote sensing, urban GIS/BIM layers, spatial weather fields, time-series + images; datasets often medium to large-scale multimodal                                            | Predominantly cloud/centralised training; inference can be centralised (planning tools) or edge-assisted (e.g., UAVs)                                          | Moderate–High                  | Fault detection in PV using UAV images and rough sets; GAN-enhanced PV grid-integration robustness; knowledge-integrated GAN for stochastic year-round PV weather time series; generative spatial AI for smart-city digital twins; AutoML-SHAP PV output prediction.                                                                                                                                                                                |
| AM-3: Deep reinforcement learning & multi-agent DRL                                  | DQN-type, PPO/actor–critic, multi-agent DRL (MADRL), DRL-based multi-objective schedulers for VPPs, smart grids and UAV swarms                                      | High-fidelity simulation environments of power systems, VPPs, EV charging and UAV networks; synthetic demand/RES data plus sampled market scenarios; data mostly simulator-generated with embedded historical traces | Decentralised/multi-agent controllers for VPPs, microgrids, and UAV-assisted EMPD; decisions executed in distributed agents with possible cloud-based training | Moderate                       | DRL-based multi-objective optimisation for VPPs and smart grids; generative AI-driven multi-agent DRL for task allocation in UAV-assisted EMPD in 6G-enabled SAGIN networks; microgrid control under transient conditions with AI-based VF controller.                                                                                                                                                                                              |
| AM-4: Hybrid physics-informed, digital-twin & surrogate models (incl. XAI)           | Physics-informed NNs, surrogate models coupled to FEM/CFD/process simulators, DT+ML pipelines, XAI-enhanced models (global–local explainable AI, SHAP, symbolic+ML) | Simulation-rich datasets from CFD, FEM, process simulation, adsorption/thermal models, and digital twins; often augmented by smaller experimental datasets for calibration                                           | Primarily centralised, embedded in design tools or digital-twin platforms; some edge-linked DTs for real-time health monitoring                                | High                           | DT + statistical ML for residential energy modelling; DT-based deep learning for personalised thermal comfort; coal-gangue concrete modelling with integrated global–local XAI and FEM; CFD + ANN–GA for solar dryers; process-simulation + AI tri-objective optimisation for DME and biomass-driven SOFC–NH <sub>3</sub> plants; digital-twin driven microgrid health management; eFILES process flowsheet synthesis combining symbolic AI and ML. |
| AM-5: Metaheuristic and evolutionary optimisation (often hybridised with ML)         | GA, PSO, bio-inspired swarm algorithms, ANN–GA hybrids, multi-objective evolutionary algorithms, heuristic search coupled to surrogates                             | Synthetic design spaces and simulation outputs (energy system models, process simulators, device models); simulation-based datasets with structured design variables                                                 | Deployment mostly within offline planning/optimisation tools; some embedded in engineering design workflows                                                    | Moderate–High                  | Metaheuristic optimisation for PEMFC performance; combined CFD + ANN–GA optimisation of solar dryers; bio-inspired AI for regenerative-braking optimisation in electric buses; nature-inspired solutions for clean-energy integration in smart grids; multi-criteria optimisation of nano-materials for EV supercapacitors; GA-style search in geothermal and district-heating designs.                                                             |
| AM-6: Classical ML & shallow ANNs for regression / classification / decision support | MLPs, random forests, gradient-boosted trees, SVM/SVR, fuzzy systems, statistical ML (e.g., logistic regression, clustering)                                        | A mix of field datasets (manufacturing energy, EV charging profiles, building stock, PV production, emissions) and experimental data (materials, devices); scales from hundreds to tens of thousands of samples      | Almost entirely centralised decision-support or analytic tools; some embedded in local EMS platforms                                                           | High                           | Energy-consumption analysis and forecasting in manufacturing; battery management with neural networks and electrochemical AI; AI-based PV cooling and dust-mitigation control; morphological classification of Italian school building stock; building-energy and GHG estimation using XAI; emission forecasting with neural computation; smart irrigation and smart-city decision support systems.                                                 |
| AM-7: AI/ICT infrastructure, accelerators and edge/federated architectures           | Hardware-oriented NN accelerators (FPGA/ASIC, photonics, STT-MRAM in-memory), resource-efficient DL, edge AI for 6G, federated                                      | Benchmarks and synthetic workloads; communication-network traces; generic ML workloads rather than domain-specific energy data; data sizes typically large-scale, matching networking or chip-level evaluation       | Edge/embedded (on-chip, EV traction inverters, IoT nodes), federated/distributed (LoRaWAN, SAGIN, 6G), and hierarchical edge–cloud deployments                 | High within ICT-focused subset | Integrated large-scale photonic accelerator with ultralow latency; co-designed silicon-photonics chip I/O for petascale connectivity; FPGA-based neural-activation accelerators; STT-MRAM in-memory computing; AI accelerators for EV BMS; edge AI for 6G; federated LoRaWAN architectures; AI-enabled integrated                                                                                                                                   |

|                                                                                                        |                                                                                                                                                                                                           |                                                                                                                  |                                                                                                                     |                                                 |                                                                                                                                                                                                                                                                                                         |
|--------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------|-------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
|                                                                                                        | learning for LoRaWAN, AI-enabled SAGIN and O-RAN                                                                                                                                                          |                                                                                                                  |                                                                                                                     |                                                 | sensing–communication–computation surveys; timing guarantees for embedded AI inference.                                                                                                                                                                                                                 |
| AM-8: Reviews, bibliometrics and conceptual frameworks (methodological synthesis rather than training) | Narrative and systematic reviews, bibliometric mapping, conceptual architectures for AI-driven energy systems; methods discussed include LSTM, CNNs, RF, DRL, GNN, DT, etc., but not trained in the paper | Training data are secondary (literature corpora, bibliographic databases) rather than curated numerical datasets | Deployment conceptual – architectures and taxonomies for future centralised, edge, federated and multi-agent AI-IES | Moderate–High (significant fraction of Table 1) | Reviews of AI in next-generation power electronics; hybrid RES (hydrogen–biomass–biogas–PV) systems; AI-driven hydrogen and battery technologies; challenges of RES integration into microgrids; bibliometric analysis of PV integration in buildings; reviews of AI-based V2X and smart-grid security. |

### 5.2.1 Supervised Deep Learning for Time-Series and Tabular Forecasting

Supervised deep learning applied to time-series and tabular data in Table 6 dominates the first cluster (AM-1), where transformer-based and recurrent models mine high-frequency operational records for probabilistic risk-aware forecasting and predictive accuracy. This trend is best illustrated by the early-stage degradation prediction in lithium-metal batteries, where stacked temporal deep networks use long-term electrochemical signatures to predict capacity loss and safety concerns prior to failure [104]. The integration of cloud-integrated residential energy management frameworks with LSTM-driven solar forecasting demonstrates how these models are implemented centrally while communicating with dispersed prosumers [105]. Regional heat-load forecasting using adversarially trained models [106] highlights the significance of robust generalisation to shifting occupancy regimes and climate. By combining weather, socioeconomic, and behavioural signals into a single temporal representation that scales to millions of samples from smart-meter fleets, multimodal feature discovery pipelines for power-demand forecasting go beyond AM-1 [107–109].

### 5.2.2 Spatial/Vision/Generative Deep Models

High-resolution thermographic imaging and advanced classifiers are utilised in UAV-based fault detection in photovoltaic plants to autonomously detect soiling, hotspots, and string failures under real operating settings [59]. In the context of photovoltaic integration, knowledge-integrated generative adversarial networks (GANs) that generate year-round stochastic weather illustrate how generative models can address deficiencies in historical data, facilitating reliability assessments and long-term capacity increase amidst climate variability [110]. Huang et al. [89] assert that generative spatial AI for sustainable smart cities facilitates scenario exploration of transportation, land use, and energy infrastructure in densely populated urban regions by integrating large-flow models with urban digital twins. AutoML frameworks utilising SHAP interpretability facilitate the autonomous exploration of designs and hyperparameters for photovoltaic power forecasts, ensuring transparency for planners and regulators, hence closing the loop [111].

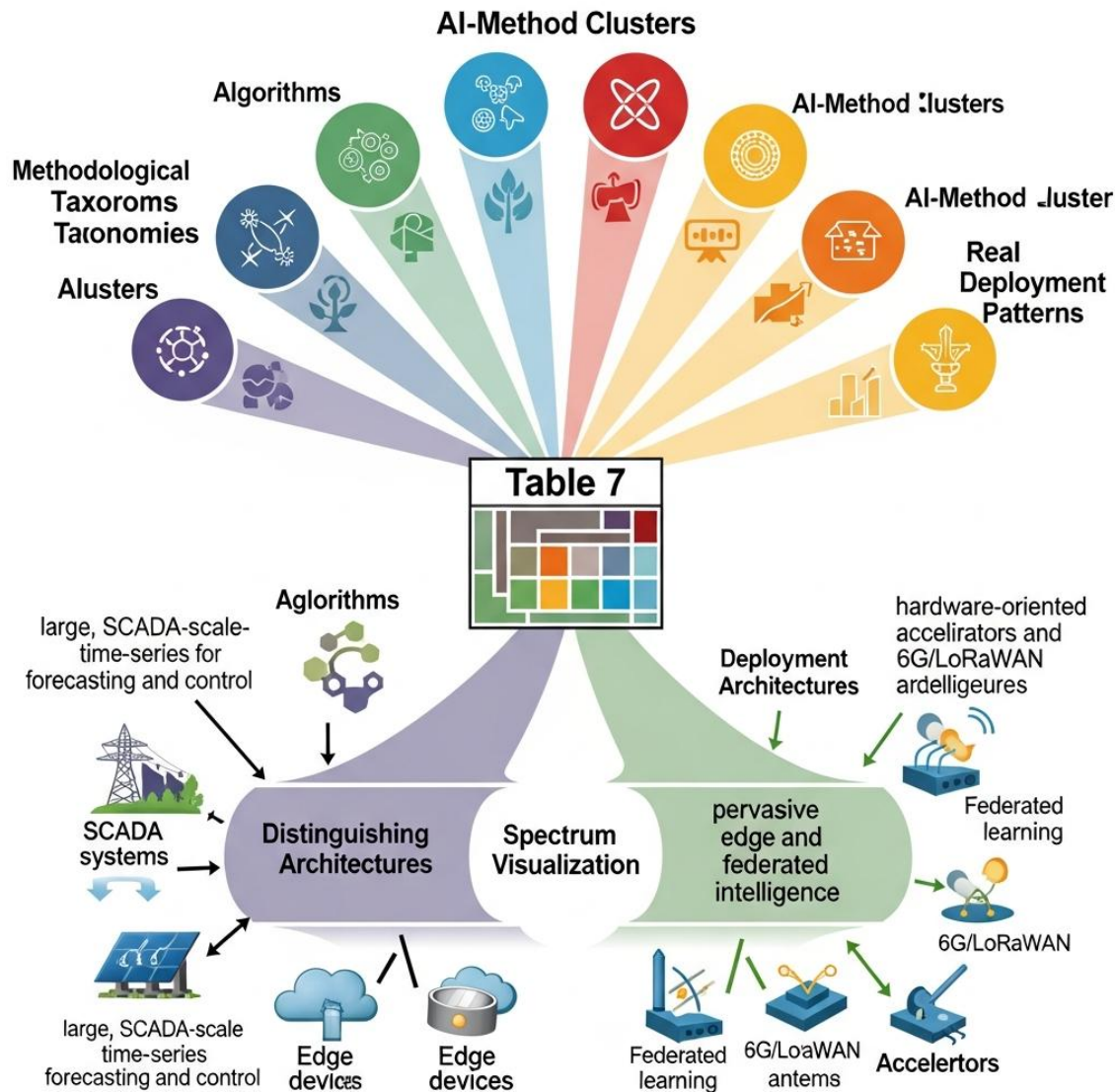


**Fig. 13.** AI-methods classification by data and deployment architecture

### 5.2.3 Deep Reinforcement Learning & Multi-Agent DRL

For real-time decision-making in intricate, multi-actor energy environments, AM-3 focuses on deep reinforcement learning (DRL) and multi-agent DRL. DRL-based multi-objective schedulers for smart grids and virtual power plants show how actor-critic and DQN-like agents can work together to maximise grid efficiency and renewable penetration in the face of unpredictable weather and price fluctuations [112]. A different frontier is demonstrated by multi-agent DRL in UAV-assisted energy-aware mobile platforms, where generative AI-driven MADRL tightly co-optimizes communication and energy budgets by coordinating swarms for task allocation within 6G-enabled space-air-ground integrated networks [113]. Artificial intelligence (AI)-based VF control schemes for isolated operation under transients demonstrate how reinforcement learning can stabilise voltage and frequency during disruptions, thereby integrating adaptive intelligence into local controllers at the microgrid level [114].

#### 5.2.4 Hybrid Physics-Informed, Digital-Twin & Surrogate Models (incl. XAI)

AM-4 teams hybrid physics-informed, digital-twin, and surrogate models, demonstrating a robust trend towards AI that honours fluid-dynamic, electrochemical, and thermodynamic structures. Digital twin plus statistical machine learning frameworks for intelligent residential energy modelling [115] demonstrate the ability to calibrate occupant-sensitive energy twins by combining high-resolution building physics simulations with measured consumption and comfort data. By embedding DL models within the twin, digital-twin-based deep learning for personalised thermal comfort in smart buildings goes one step further in adapting HVAC operation across diverse occupants and climate conditions [115]. For coal-gangue concrete constitutive modelling, global–local explainable AI combined with FEM is an example of surrogate modelling, in which interpretable AI approximates physics-based simulations to allow for quick but traceable structural evaluations [116]. The ability of hybrid pipelines to search large design spaces in integrated power–fuel systems while meeting multi-criteria performance targets is demonstrated by the tri-objective optimisation of biomass-driven SOFC–ammonia plants based on process simulation with AI-assisted surrogates [62, 117].

#### 5.2.5 Metaheuristic and Evolutionary Optimization (often hybridized with ML)

AI-enhanced search over high-dimensional design and operating spaces, frequently hybridised with ML surrogates to lessen computational burden, is what defines the metaheuristic and evolutionary optimisation cluster (AM-5). AI-driven modelling and metaheuristic optimisation for improved PEM fuel-cell performance demonstrate how evolutionary algorithms traverse nonlinear parameter landscapes of membrane hydration, operating temperature, and gas stoichiometry to increase efficiency and durability [45]. To redesign geometries for household-scale applications, the combined CFD and ANN–GA optimisation of direct solar dryers similarly combines neural surrogates, genetic algorithms, and high-fidelity airflow and thermal models [118]. Electric buses' bio-inspired AI-tuned regenerative braking demonstrates how swarm-based heuristics can be used to find control schemes that balance battery life, passenger comfort, and urban energy recovery [91]. Algorithms that support multi-objective planning across resilience, cost, and emissions dimensions are further demonstrated by nature-inspired optimisation of smart-grid integration strategies [119].

#### 5.2.6 Classical ML & Shallow ANNs for Regression/Classification/Decision Support

In areas where interpretability is important or data volumes are low, such as decision support, diagnostics, and moderate-scale forecasting, AM-6 combines traditional machine learning and shallow artificial neural networks. For instance, ML-based analysis of consumption histories is used in case-study-based energy management in German manufacturing to find opportunities for demand-shifting and retrofitting without the need for specialised hardware or deep models [120]. Without the burden of massive DL models, neural-network-based battery management frameworks integrate electrochemical AI surrogates for state-of-charge and state-of-health estimation into BMS controllers [121]. To optimise water and energy efficiency in agricultural settings, smart irrigation systems driven by solar photovoltaics and the Internet of Things use classical machine learning classifiers and regressors to schedule water delivery under soil moisture and climate constraints [122]. Explainable AI-based building energy and GHG estimation

shows how feature attribution techniques and gradient-boosted trees can help policy-compliant retrofitting choices for a variety of building stocks [56, 123-125].

### 5.2.7 AI/ICT Infrastructure, Accelerators and Edge/Federated Architectures

By moving inference to silicon-photonics fabrics, integrated photonic accelerators with ultralow latency meet the computational demands of large DL models and allow on-chip processing for high-throughput applications [126]. The tight co-optimization of communication and computation infrastructures that will support future AI-embedded grids and mobility networks is indicated by co-designed silicon-photonics chip I/O for petascale connectivity and photonic hybrid beamforming for 5G/6G millimetre-wave systems [127, 128]. Further indicating a move towards ultra-efficient on-device AI appropriate for EV traction inverters and embedded controllers are FPGA-based neural-activation accelerators and STT-MRAM in-memory computing architectures [129, 130]. Distributed learning is integrated into far-edge IoT for energy and environmental monitoring through federated LoRaWAN architectures and edge AI for 6G, allowing for privacy-preserving analytics across massive sensor fleets [68, 131, 132].

## 5.2. Reviews, Bibliometrics and Conceptual Frameworks

Last but not least, AM-8 gathers reviews, bibliometrics, and conceptual frameworks that influence future data and deployment architectures across all other clusters without actually training models. A cross-cutting synthesis of algorithm selections, device constraints, and control strategies drawn from the review of recent AI applications in next-generation power electronics informs hardware co-design and controller choice [1]. A thorough analysis of solar-PV hybrid renewable systems, biomass, hydrogen, and biogas identifies gaps in AI techniques for sector coupling and long-duration storage while mapping optimisation and control strategies across multi-vector portfolios [64]. The successful deployment of AI depends not only on model performance but also on strong data governance, cyber-physical security, and regulatory alignment, according to thorough reviews of integration challenges in microgrids and AI-driven hydrogen and battery technologies, respectively [133, 48]. The idea that deployment architecture and data availability co-evolve with policy incentives and innovation trajectories is supported by bibliometric mapping of PV integration in buildings, which also establishes the agenda for the upcoming generation of AI-driven integrated energy systems (Elaziz Waseef, A.A.) [134, 135].

## 5.3 Functional-Role Matrix for AI-Driven Integrated Energy Systems

Forecasting and situation awareness functions compile the body of work that transforms unprocessed time-series and environmental data into predictive signals for dispatch and infrastructure readiness. Advanced load and heat prediction frameworks using adversarially trained models have shown that data-driven architectures are now able to capture non-linear demand-weather interactions at the regional scale, allowing for more resilient planning under climate variability [106]. By creating realistic future irradiance trajectories for PV integration analysis, generative time-series models for stochastic weather synthesis go beyond this, transforming uncertainty from a risk externality into a structured design input [110]. These forecasts are integrated into real-time decision engines that co-optimize renewable penetration, grid efficiency, and multi-objective performance metrics by deep reinforcement learning controllers for virtual

power plants and smart grids at the operational frontier [112]. Incorporating such models into production EMS pipelines results in quantifiable improvements in cost, efficiency, and forecast-driven operations, according to case-study evidence from industrial energy management [120].

Table 7's second pillar consists of planning, sizing, and multi-vector techno-economic optimisation, which translates AI-enhanced insight into sector-coupled architectures and structural investment decisions. According to Taghavi et al. [2], coordinated energy management studies for multi-vector systems combine electricity networks, underground gas storage, and maritime scheduling within an AI-supported optimisation framework, showing how system-wide costs and emissions can be decreased concurrently while taking advantage of cross-vector synergies. Integrated gasification fuel cell systems with carbon capture in high-efficiency, low-carbon power plants extend this logic, where AI-guided gradient utilisation across thermal and electrochemical stages promotes enhanced techno-economic performance and carbon reduction [79]. The co-production of electricity and ammonia by biomass-driven solid oxide fuel cell complexes foreshadows future hydrogen–ammonia corridors by demonstrating how AI-based tri-objective optimisation can balance economic, energetic, and environmental criteria in power-to-X chains [62]. A meta-level lens is added by systematic reviews of hybrid hydrogen, biomass, biogas, and PV portfolios, which map the areas where integration barriers are still at the planning scale and where AI has the biggest marginal impact in hybrid configurations [64].

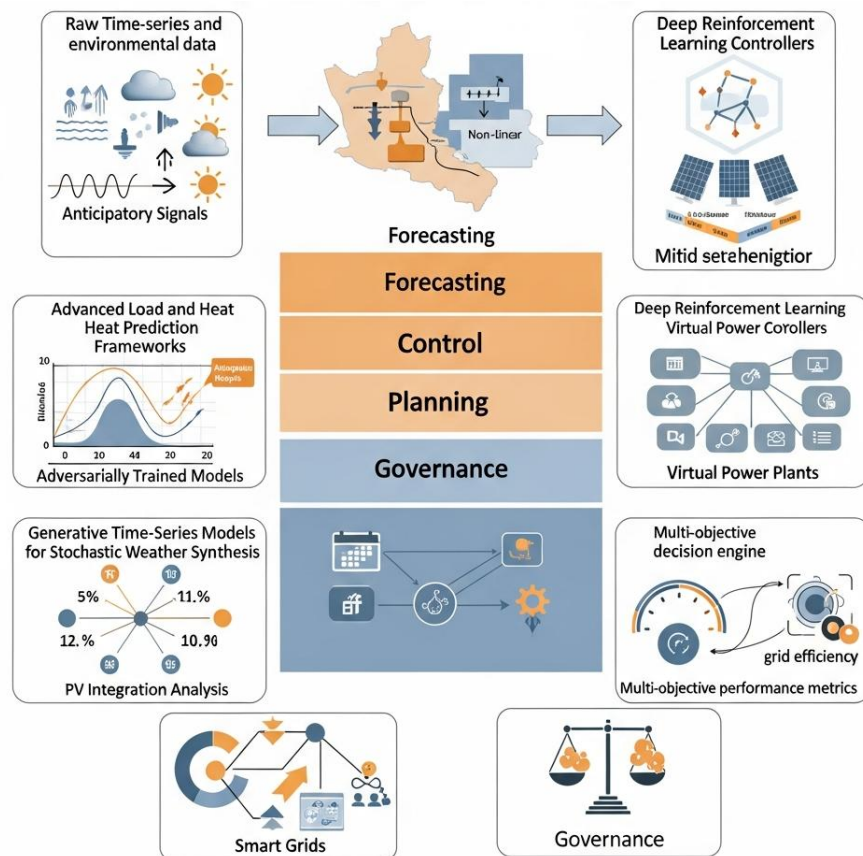


**Fig. 14.** Functional-role matrix for AI-Driven Integrated Energy Systems

Effectively integrating intelligence at the hardware and component level, a third cluster of functional roles in Table 7 is centred on diagnostics, materials or component co-design, and asset health. For lithium-metal batteries, stacked temporal deep learning models are an example of how early inference of fine-grained degradation trajectories can facilitate safer deployment of high-energy-density chemistries in stationary or mobile systems, predictive maintenance, and operating window redesign [104]. By combining computer vision, drones, and AI planners, autonomous robotics for PV cleaning and predictive maintenance transform soiling and fault detection into a continuous, minimally human-supervised process that stabilises PV yield and lowers O&M costs [44]. Further, by incorporating rough-set theory into AI-based fault classifiers, UAV-based thermal and visual inspection frameworks increase sensitivity to early-stage module degradation and hotspot formation [59]. Neural-network-assisted numerical modelling for advanced solar panels speeds up the investigation of geometry-material-performance trade-offs by compressing costly CFD or electromagnetic simulation loops into surrogate models [44]. The trend for functional fluids is similar to that of optimising MXene-based aqueous ionic liquids for solar systems, where electrolytes with superior conductivity and stability profiles are obtained through AI-guided search over composition space [46].

The matrix also emphasises human-centric functional roles that are closely related to developing sensing and communication infrastructures, particularly in the areas of buildings, comfort, and urban systems. According to Almadhor et al. [4], digital twin frameworks for residential and commercial buildings demonstrate how deep learning can be combined with occupancy and indoor environmental data to provide individualised thermal comfort while lowering HVAC energy consumption, thereby transforming each building into a self-calibrating cyber-physical system. Planners can identify renovation archetypes and prioritise deep retrofits where energy savings and emissions reductions are greatest by classifying the building stock at the urban scale using AI-supported morphological analysis [87]. Studies on carbon-neutral tropical buildings show that in environments where latent and sensible loads are closely coupled, AI-optimized comfort control can yield notable efficiency gains [86]. According to surveys of AI-enabled integrated sensing, communication, and computation, these applications heavily depend on reliable sensing and communication backbones. For future SAGIN and 6G environments, signal processing, machine learning, and network protocols must be co-designed [19]. Resource-efficient federated LoRaWAN architectures and AI-augmented SAGIN solutions show that dense urban and regional energy observatories require far-edge IoT devices to participate in distributed analytics without overloading network or energy budgets [68, 136, 137].

Table 7 lists governance, security, and resilience as cross-cutting protections for increasingly self-governing AI–energy ecosystems. According to ML-based smart grid intrusion detection studies, cyber anomalies can be identified almost instantly from SCADA and network traces, lowering the possibility that hostile manipulation of AI controllers or sensor streams will result in physical disruptions [98]. Integrative reviews of blockchain and AI for safe smart grids broaden this perspective by taking decentralised control, integrity, and non-repudiation into account, especially when PV and EV penetration is high [69]. Broader critical infrastructure analyses highlight how integrating AI systems at scale can increase attack surfaces and systemic vulnerabilities if not coupled with strong governance and resilience design [70] by recasting AI as a dual-use capability requiring strict safeguards. Work on Germany's energy security plan during the Russian gas exit shows how environmental policy and AI-augmented energy systems co-

evolve under geopolitical stress, with digital tools guiding decarbonisation trajectories, risk hedging, and diversification pathways [102]. Complementary analyses of the economic, social, and regulatory aspects of AI-driven smart buildings highlight the need for adaptive regulation that can keep up with the rapid digitalisation of smart buildings while preserving data rights, privacy, and equity [138]. Last but not least, Table 7 includes knowledge synthesis and roadmapping roles that match long-term trajectories for AI-driven integrated energy systems with the scattered technical advancements. In-depth analyses of AI in next-generation power electronics outline the device-level and algorithmic advancements required to support multi-vector interfaces and highly dynamic, converter-rich grids, thereby establishing baseline capabilities for upcoming hardware platforms that support AI [1]. AI has gradually moved from peripheral optimisation tasks to central roles in design, performance forecasting, and lifecycle assessment, according to bibliometric analyses of building-integrated photovoltaics conducted between 1971 and 2025 (Elaziz Waseef, A.A.). In the context of the developing hydrogen economy, reviews of AI-driven battery and hydrogen technologies synthesise developments in materials, systems, and control layers, elucidating the ways in which AI offers revolutionary improvements in storage, conversion, and utilisation [48]. Systematic evaluations of AI-powered carbon capture and biomass-to-bioenergy technologies place these advancements within larger carbon-neutrality roadmaps, exposing competition and complementarities between various negative-emission and circular-energy approaches [139]. The functional-role matrix transforms the 153-reference corpus into a strategic map by placing these synthesis studies next to forecasting, operations, planning, and security functions. This demonstrates how layered AI capabilities, from embedded devices to policy dashboards, can be coordinated into cohesive, resilient, and equitable energy transitions.

**Table 7.** Functional-role matrix for AI–Driven Integrated Energy Systems

| Function<br>al Role<br>ID | Functional<br>Focus in<br>Integrated<br>Energy<br>Systems                                                                                                            | Dominant<br>System<br>Layers /<br>Assets                                                               | Typical Data<br>Streams                                                                                                      | Key AI / Analytics<br>Approaches                                                                                               | Primary<br>Performance<br>/ Policy<br>Outcomes                                                                                                                     | Representati<br>ve Studies<br>from<br>Corpus*                                                                                   |
|---------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------|
| FR-1                      | Forecasting<br>& Situation<br>Awareness –<br>anticipatory<br>intelligence<br>for demand,<br>generation,<br>weather, and<br>thermal loads<br>in integrated<br>systems | Distribution<br>grids, district<br>heating/cooling,<br>building<br>clusters,<br>regional load<br>zones | High-frequency<br>SCADA time-<br>series, smart-meter<br>data,<br>meteorological and<br>climate series,<br>occupancy profiles | Supervised DL<br>(LSTM, CNN,<br>transformers),<br>adversarially trained<br>predictors, feature-<br>engineered ML<br>regression | Improved<br>forecasting<br>accuracy for<br>load/heat,<br>enhanced<br>reserve<br>planning,<br>reduced<br>imbalance<br>penalties,<br>climate-<br>robust<br>operation | Zhu et al.<br>[106] –<br>regional heat-<br>load<br>forecasting<br>with<br>adversarially<br>trained data-<br>driven<br>models    |
| FR-2                      | Real-Time<br>Operations &<br>Energy/Power<br>Management<br>– closed-loop<br>control of<br>VPPs,<br>microgrids,<br>and EV<br>ecosystems                               | Microgrids,<br>VPPs, smart<br>EV charging<br>hubs, grid-tied<br>PV–BESS–H <sub>2</sub><br>systems      | Real-time power<br>flows, price<br>signals, SoC/SoH,<br>congestion and<br>frequency<br>indicators                            | Deep reinforcement<br>learning, hybrid rule-<br>based + DRL EMS,<br>multi-objective<br>control optimisers                      | Maximised<br>renewable<br>integration,<br>reduced<br>curtailment,<br>improved<br>grid<br>efficiency<br>and<br>flexibility,<br>cost-optimal                         | Tang &<br>Wang [112] –<br>DRL-based<br>multi-<br>objective<br>optimisation<br>for virtual<br>power plants<br>and smart<br>grids |

|      |                                                                                                                            |                                                                                                                            |                                                                                                              |                                                                                                                       |                                                                                                                           |                                                                                                                                        |
|------|----------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------|
|      |                                                                                                                            |                                                                                                                            |                                                                                                              |                                                                                                                       | dispatch                                                                                                                  |                                                                                                                                        |
| FR-3 | Planning, Sizing & Techno-Economic Optimisation – strategic configuration of multi-vector infrastructures                  | National or regional multi-vector systems, underground storage, PtX hubs, integrated IGFC/CCS plants                       | Long-horizon demand scenarios, technology cost curves, resource profiles, regulatory and tariff data         | Scenario-based techno-economic optimisation, AI-assisted multi-criteria decision analysis, evolutionary design search | Cost-effective multi-vector integration, optimised CAPEX/OPEX, robust investment pathways under uncertainty               | Taghavi et al. [2] – techno-economic assessment for coordinated multi-vector energy management with AI-based scheduling                |
| FR-4 | Asset Health Monitoring, Diagnostics & Predictive Maintenance – reliability-centred intelligence for critical components   | Lithium-metal batteries, PV modules and strings, marine hybrid systems, rotating machinery                                 | Degradation trajectories, partial discharge and vibration signals, thermal imagery, operational profiles     | Stacked temporal DL models, anomaly detection, PHM pipelines, UAV-enabled computer vision                             | Early-stage fault detection, extended asset lifetimes, reduced unplanned outages, risk-aware maintenance planning         | Jawad et al. [104] – stacked temporal deep learning for early-stage degradation forecasting in lithium-metal batteries                 |
| FR-5 | Design & Materials / Component Co-Design – AI-guided exploration of devices, fluids, and architectures for energy hardware | Advanced PV modules, MXene-based electrolytes, geothermal fractures, adsorption chillers, aero-thermal components          | High-fidelity simulation outputs (CFD, FEM), lab-scale experiments, compositional and structural descriptors | Surrogate modelling with ANN, hybrid physics–ML meta-models, metaheuristic and GA-driven design space exploration     | Higher energy conversion efficiency, thermal stability, reduced material usage, faster design cycles                      | Mamodiya et al. [60] – numerical modelling and neural network optimisation for advanced solar panel efficiency                         |
| FR-6 | Human-Centric Comfort, Buildings & Urban Systems – socio-technical optimisation in built and urban environments            | Smart buildings, campuses, school building stock, urban districts and smart cities                                         | Indoor temperature/humidity, occupant comfort feedback, building morphology, mobility and land-use data      | Digital twins with DL, statistical ML, morphological classification, generative spatial AI                            | Energy-efficient comfort control, deep renovation roadmaps, carbon-neutral urban planning, reduced GHG from buildings     | Almadhor et al. [4] – digital twin-based deep learning framework for personalised thermal comfort and energy-efficient smart buildings |
| FR-7 | Sector Coupling & Power-to-X (PtX) Integration – cross-vector coordination of electricity, hydrogen, fuels, water and heat | Biomass-driven SOFC plants, electricity–ammonia systems, solar-driven H <sub>2</sub> production, water–energy nexus assets | Process simulations, fuel-cell operating data, feedstock flows, multi-vector energy and mass balances        | AI-assisted tri-objective optimisation, ML surrogates for process units, multi-vector techno-economic analysis        | Co-optimised electricity and fuel production, improved round-trip efficiencies, reduced lifecycle emissions in PtX chains | Dou et al. [62] – AI-based machine-learning-assisted tri-objective optimisation of biomass-driven SOFC electricity and ammonia plant   |
| FR-8 | Cyber-Physical Security, Intrusion                                                                                         | Smart grids, microgrids, IoT-rich substations,                                                                             | Network traffic logs, SCADA/PMU streams, cyber-                                                              | Supervised/unsupervised ML for IDS, anomaly detection, AI-driven cyber-risk                                           | Early detection of cyber-attacks, enhanced                                                                                | Abou-Elasaad et al. [98] – smart grid intrusion                                                                                        |

|       |                                                                                                                                    |                                                                                                                        |                                                                                                   |                                                                                                                |                                                                                                                               |                                                                                                                              |
|-------|------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------|
|       | Detection & Resilience – safeguarding digitalised energy infrastructures                                                           | critical infrastructure with AI-enabled controls                                                                       | event traces, IDS signatures, operational states                                                  | analytics                                                                                                      | resilience of autonomous control, reduced vulnerability of critical infrastructures                                           | detection system based on AI techniques                                                                                      |
| FR-9  | Policy, Governance & Market Design Intelligence – linking AI-driven systems to strategic energy security and regulatory frameworks | National energy systems, gas and electricity markets, city-level solar policies, smart-building regulation             | Macroeconomic indicators, policy scenarios, technology roadmaps, deployment statistics            | Policy-oriented modelling with AI insights, data-driven decision support frameworks, explainable analytics     | Informed energy security strategies, accelerated renewable deployment, evidence-based regulation and incentives               | Salman [102] – analysis of Germany’s AI-driven energy systems within an energy security strategy during the Russian gas exit |
| FR-10 | Sensing, Communication & Edge-Intelligence Infrastructure – AI-ready connectivity for distributed energy assets                    | Edge devices, 5G/6G SAGIN, LoRaWAN sensor networks, integrated sensing–communication–computation platforms             | Multi-modal sensor data, RF/optical channel metrics, device telemetry, embedded compute workloads | Integrated sensing/communication on AI, federated learning at the edge, AI-enabled network resource management | Low-latency and energy-efficient data transport, scalable edge analytics, enhanced observability of distributed energy assets | Wu et al. [19] – survey of AI-enabled integrated sensing, communication, and computation architectures                       |
| FR-11 | Knowledge Synthesis, Benchmarking & Roadmapping – meta-level intelligence shaping future AI–energy integration                     | Cross-domain power electronics, hybrid RES portfolios, hydrogen and battery technologies, PV integration bibliometrics | Literature corpora, patent databases, bibliometric indicators, technology performance benchmarks  | Systematic reviews, bibliometric analysis, cross-domain taxonomies, conceptual roadmapping                     | Identification of research gaps, standardisation needs, and next-generation AI–energy convergence trajectories                | Safari et al. [1] – review of AI applications in next-generation power electronics guiding technology evolution              |

#### 5.4 Objective–Constraint Classification of AI–IES

The techno-economic cluster includes research that maximises efficiency and utilisation while minimizing cost metrics like LCOE and LCOH, as shown in Table 8 and Fig. 15. This is frequently accomplished through multi-objective optimisation that combines AI surrogates with physics-based models. Ayadi et al. [45] use proton-exchange membrane fuel cell modelling to illustrate this pattern, which uses AI-driven metaheuristics to manage stack performance and operating cost trade-offs. Similar formulations can be found in multi-vector systems that manage maritime logistics and subterranean storage, where Taghavi et al. [2] employ AI-based scheduling to minimise system-wide costs while adhering to infrastructure and tariff constraints. Li et al.'s (2025) optimisation of integrated gasification fuel cells with carbon capture in advanced thermochemical systems under synergistic energy-gradient constraints demonstrates how the economic goals in Table 8 are closely tied to market regulations, emissions caps, and hardware limitations.

**Table 9.** Objective–constraint classification of AI–IES

| Objective–constraint cluster (ID)                             | Brief description of optimisation focus                                                                                                 | Dominant system-level objectives in AI–IES                                                                                                                                                                                              | Typical constraint sets encoded in models                                                                                                                                                                                                                                               | Evidence density                                                                                                     | Representative AI / data methods emphasised                                                                                                                                                                                    | Illustrative application domains & exemplar studies*                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
|---------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| A. Cost, techno-economic performance and efficiency           | Economic and performance-driven formulations that trade off CAPEX/OPEX, efficiency and resource utilisation in integrated energy assets | Minimise investment and operating cost, LCOE/LCOH/LCOX; maximise conversion efficiency, utilisation factors and profitability; perform multi-objective cost–performance trade-offs at component, system and infrastructure scales       | (C1) Device/network limits: converter ratings, PEMFC current density windows, battery SoC and thermal limits; (C2) tariff schemes, incentive structures and investment budgets; (C3) occasionally climate/resource scenarios for long-term planning                                     | High – largest and most mature cluster, covering TES, microgrids, industrial parks and hydrogen value chains         | Metaheuristic optimisation (GA/PSO and hybrids), evolutionary multi-objective optimisation, ANN-GA surrogates, deep temporal networks and ML-assisted techno-economic solvers (e.g., PEMFC and IGFC/CCS optimisation) [45, 79] | Multi-vector techno-economic scheduling with underground storage and maritime logistics [2]; solar dryers and trackers tuned via CFD-ANN and ANN-GA metaheuristics [118, 76]; CSP with storage optimised using AI models [170]; geothermal cooling/power cycles and fractured geothermal systems designed via ML-assisted multi-objective frameworks [43, 179]; Mega-DIP petrochemical park decarbonisation and energy system sizing under generative-AI techno-economics [24].                                                            |
| B. Emissions reduction, carbon neutrality and circularity     | Environmental and circular-economy-driven formulations targeting net-zero, low-carbon and resource-circular operation                   | Minimise lifecycle GHG emissions and carbon intensity; enforce net-zero and carbon-neutral operation; maximise resource circularity across water, biogas, biomass, PV and industrial processes                                          | (C3) Explicit environmental targets: net-zero roadmaps, carbon budgets, water–energy nexus and circularity constraints; (C1) technical feasibility of CCUS, biomass/biogas and PV/renewable integration; (C2) policy standards, environmental regulations and sustainability benchmarks | Moderate–High – concentrated around water sector, buildings, biomass/biogas, hydrogen and industrial decarbonisation | Supervised and hybrid ML for emissions estimation, XAI for carbon attribution, optimisation-driven process integration, AI-supported CCUS system design and generative AI for scenario exploration [17, 56]                    | AI-optimised biogas production in water resource recovery facilities to achieve carbon-neutral operation [17]; carbon-neutral tropical buildings with AI-optimised comfort and energy control [86]; net-zero water-sector case studies [82]; biomass-to-bioenergy pathways with AI-assisted CCUS [139]; building energy consumption and GHG estimation using explainable AI [56]; low-emission smart-city mobility architectures [94]; generative-AI-assessed decarbonised petrochemical industrial parks [24].                            |
| C. Flexibility, scheduling and multi-vector energy management | Flexibility-centric formulations that schedule multi-vector resources and loads under uncertainty and high renewable penetration        | Maximise renewable utilisation and self-consumption; minimise curtailment; optimise dispatch of hybrid PV–FC–BESS–H <sub>2</sub> and EV fleets; support V2G/V2X and virtual power plant (VPP) participation while maintaining stability | (C1) Power-flow feasibility, microgrid stability margins, SoC limits, ramping and charging rate constraints; (C2) market rules: TOU tariffs, ancillary service remuneration, VPP participation limits; (C3) weather-driven variability and stochastic demand                            | High – one of the densest clusters, spanning microgrids, EV/charging, hybrid RES and smart-city operations           | DRL-based multi-objective optimisation, model-predictive control with learned surrogates, probabilistic ML for scenario generation, ANN-based forecasting and hybrid rule-based/ML controllers [112, 18]                       | Multi-layer AI optimisation for grid-tied PV–fuel cell hybrid systems [15]; DRL-enabled VPP and smart-grid dispatch to maximise renewable integration [112]; probabilistic energy management of hydrogen-integrated microgrids with V2G [18]; AI-driven smart EV charging coupled with PV and BESS in dense residential settings [90]; IoT-driven intelligent energy management in buildings and neighbourhoods [140]; reviews and controllers for microgrid integration challenges and redox-flow battery frequency regulation [133, 77]. |

|                                                                  |                                                                                                                                                    |                                                                                                                                                                                                                   |                                                                                                                                                                                                                                                                                |                                                                                                          |                                                                                                                                                                                                                                |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
|------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| D. Reliability, security and power quality                       | Safety- and security-oriented formulations that protect critical assets, maintain power quality and guard against cyber-physical threats           | Maximise reliability indices and asset health; minimise fault incidence, false alarms and outage durations; ensure voltage/frequency quality and secure operation of cyber-physical energy infrastructures        | (C1) Protection, stability and PQ limits (voltage, frequency, THD, device stress); (C2) cyber-security policies, intrusion-detection thresholds and compliance rules; (C3) hazard scenarios such as fire risk, maritime navigation uncertainty and component degradation paths | Moderate – focused but pivotal for critical infrastructure and high-risk environments                    | Deep anomaly detection and intrusion-detection networks, CNN/vision-based fault detection, DT-enabled health management, PHM models, hybrid ML for PQ assessment and explainable models for safety-critical decisions [98, 51] | Reliability assessment of autonomous maritime navigation systems under uncertainty [146]; AI-based smart-grid intrusion detection frameworks [98]; UAV- and AI-enabled fire-hazard detection in PV plants [141]; digital-twin-driven health management for microgrids [65]; UAV-image-based PV fault detection using rough-set theory [59]; power-quality assessment in grid-connected PV systems via deep learning [78]; prognostics and health management for marine hybrid energy systems [51].                                                                                              |
| E. Resilience and risk under disturbances                        | Strategic-risk and resilience formulations for shocks such as supply disruptions, climatic extremes and cyber or infrastructure attacks            | Enhance resilience to exogenous shocks, reduce recovery time and unserved energy, support energy-security objectives, maintain service continuity under extreme or hostile conditions                             | (C3) Exogenous hazards and shocks: geopolitical gas supply disruption, extreme weather, maritime and communication risks; (C1) infrastructure robustness, redundancy and islanding limits; (C2) high-level security and resilience policy frameworks                           | Nascent– Moderate – fewer studies but high strategic importance for planning and policy                  | Robust and adversarial ML for forecasting under perturbations, scenario-based optimisation, risk-aware control, graph-based resilience metrics and AI-augmented stress-testing of critical systems [106, 136]                  | AI-driven framing of Germany's energy security strategy during the Russian gas exit [102]; critical-infrastructure vulnerability analyses under accelerated AI integration [70]; SAGIN- and maritime-network-enabled resilient communication for energy and logistics [136, 67, 113]; adversarially robust regional heat-load forecasting for district heating and buildings [106]; resilience-oriented biomass-to-bioenergy and CCUS planning under net-zero constraints [139].                                                                                                                |
| F. Comfort, service quality and user-centric performance         | Human-centric formulations that embed comfort, accessibility and service quality in energy control problems                                        | Maximise thermal and visual comfort, indoor environmental quality, mobility service quality and accessibility; support healthcare, assistive technologies and user-experience metrics alongside energy efficiency | (C1) Comfort ranges and QoS bounds (temperature, humidity, air quality, latency); EV ride quality and drivability; (C2) building codes, mobility and healthcare service standards; (C3) local climate, occupancy, travel and usage patterns                                    | Moderate – concentrated in smart-building, mobility and assistive-technology studies                     | Deep learning and DT-based comfort models, reinforcement learning for comfort-energy co-optimisation, edge AI for assistive systems, multi-modal sensing and preference-aware controllers [4, 158]                             | Digital-twin-based deep-learning frameworks for personalised thermal comfort and energy-efficient smart buildings [4]; AI-optimised comfort control in carbon-neutral tropical buildings [86]; regenerative-braking optimisation in electric buses for energy-efficient yet comfortable urban mobility [91]; energy-aware IoT architectures for low-emission smart-city transport [94]; edge-inference assistance systems improving accessibility for visually impaired runners [158]; AI-integrated MANET frameworks for scalable, secure healthcare IoT (Venkata Krishna Reddy et al. [205]). |
| G. Cross-cutting AI/ICT enablers with implicit energy objectives | ICT and AI-hardware-focused formulations that enable low-latency, low-energy AI, pervasive sensing/communication and AI-accelerated design/control | Minimise inference latency and computational energy; maximise throughput and reliability of sensing–communication–computation stacks;                                                                             | (C1) Hardware and protocol limits (FPGA/ASIC timing, ADC/branch predictor constraints,                                                                                                                                                                                         | High – many works primarily target AI/ICT infrastructure while implicitly enabling AI–IES deployment and | Edge-AI and AI-accelerator architectures (FPGA, STT-MRAM, neuromorphic and photonic), integrated                                                                                                                               | Edge AI for 6G and integrated sensing/communication/computation [19]; photonic accelerators and co-designed photonics chip I/O for energy-efficient petascale connectivity [126, 127, 207, 128]; FPGA-based and in-memory AI accelerators for EV battery                                                                                                                                                                                                                                                                                                                                        |

|  |  |                                                                                                            |                                                                                                                                                                                         |         |                                                                                                                           |                                                                                                                                                                                                                                                                                                   |
|--|--|------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------|---------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
|  |  | provide AI platforms and accelerators that indirectly improve energy-system monitoring, control and design | 6G/O-RAN capacities, photonic link budgets); (C2) ICT standards, interoperability and QoS; (C3) sometimes explicit energy-efficiency and sustainability criteria for ICT infrastructure | scaling | sensing–communication–computation, GAN-based synthetic data and AI-accelerated materials/device discovery [131, 206, 142] | management and medical imaging [150, 129, 208]; SAGIN and LoRaWAN architectures for far-edge IoT in energy and mobility [209, 68, 192]; GAN-based stochastic weather synthesis for PV integration [110]; AI-accelerated platforms for emerging PV materials and electro-optic devices [142, 206]. |
|--|--|------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------|---------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|

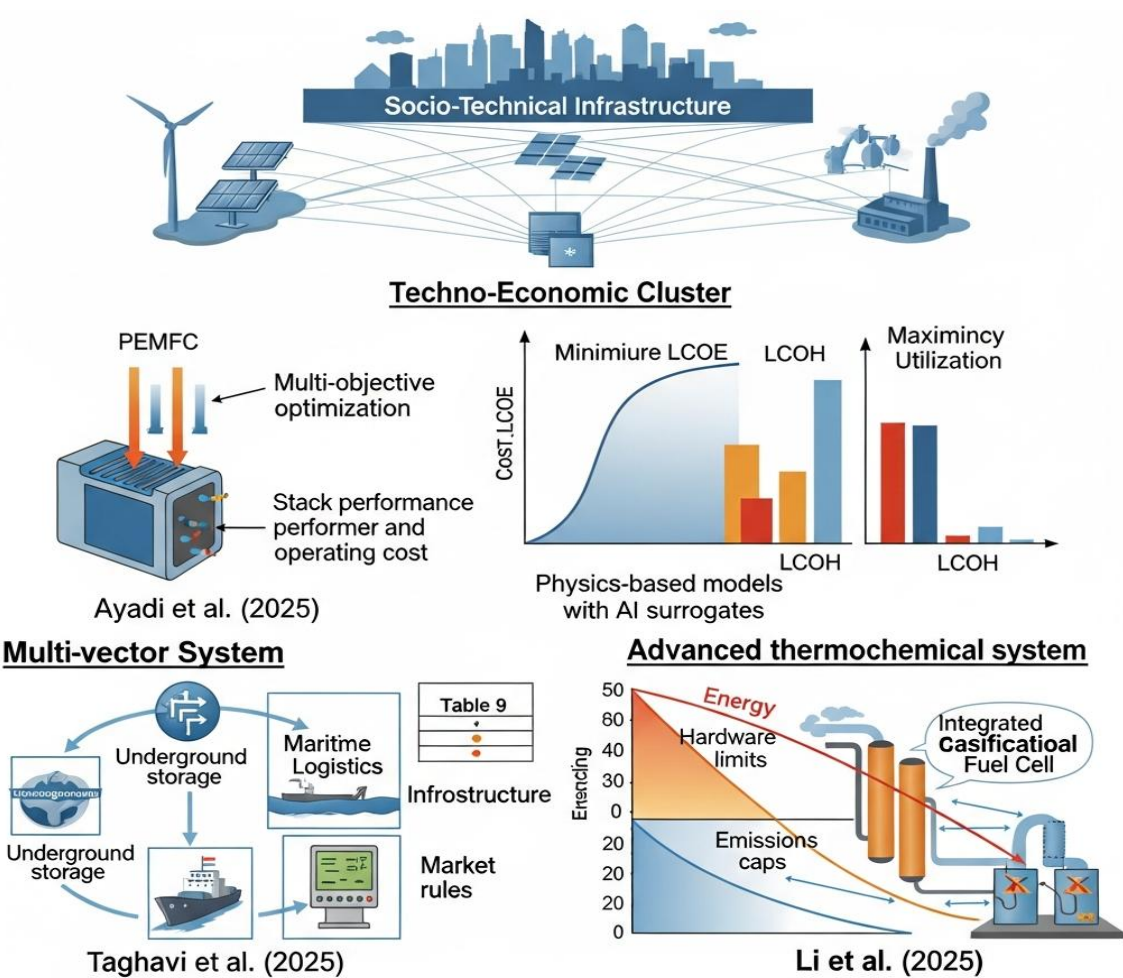


Fig. 15. Objective–constraint classification classification of AI–IES

Farzin et al. [17] develop AI-driven biogas optimisation in water resource recovery facilities to improve energy circularity under carbon-neutrality constraints, connecting lifecycle emissions limits to process-level decisions. According to Ramos et al. [82], AI-supported optimisation must meet sectoral carbon budgets and operational performance goals To achieve net-zero water-sector objectives within a case-study framework. Zhang et al. [56] estimate building energy consumption and related GHG emissions at the building and city scales using explainable AI. This allows planners to

impose explicit emissions caps and renovation targets in optimisation problems. Kim et al. [86] demonstrate the dual environmental–service nature of the objective–constraint structure in carbon-neutral tropical buildings by demonstrating how comfort-oriented controllers are limited by both indoor environmental quality and decarbonisation goals.

Another dense cluster in Table 8 is made up of flexibility, dispatch, and multi-vector scheduling. Nene and Thankachan [15] develop a multi-layer AI optimisation framework for grid-tied PV–fuel cell hybrids, encoding grid codes, fuel cell limits, and converter ratings constraints while aiming for efficiency and self-consumption goals. According to Tang and Wang [112], deep reinforcement learning for virtual power plants views grid efficiency and renewable integration as complementary goals that are subject to market participation regulations, power-flow feasibility, and SoC restrictions. Khosravi et al. [18] extend this reasoning to hydrogen-integrated microgrids with vehicle-to-grid services, where probabilistic energy management must deal with renewable variability and stochastic demand while maintaining reliability. In their AI-IES formulations, Sarker et al. [90] and Mohamed et al. [140] integrate EV charging, PV, BESS, and smart-building loads at the urban edge. This approach respects network, tariff, and comfort constraints while simultaneously optimising economic, flexible, and user-centric goals.

Table 8's objective-constraint landscape gains a safety-critical dimension from reliability, security, power quality, and resilience. According to Abou-Elasaad et al. [98], smart-grid intrusion detection prioritises security and false-alarm rates while adhering to grid protection limits and cyber-security policy constraints. Lysyi et al. [141] developed the integrated UAV-AI-SCADA method for fire hazard detection in solar power plants, which maximises risk minimization and early detection under operational and sensing constraints. According to Ebrahimi et al. [65], digital twin-driven health management in microgrids aims to reduce downtime and improve asset reliability while respecting operational, electrical, and thermal constraints. In regional heat-load forecasting under adversarial training, Zhu et al. [106] optimise forecast robustness subject to extreme-weather scenarios and district-heating constraints, exhibiting a resilience-oriented variant of these formulations. At the national level, Sambucci et al. [70] point out how accelerated AI integration can increase vulnerability surfaces and thereby introduce new security constraints into AI-IES design, while Salman [102] views Germany's energy security strategy around AI-driven systems as a resilience optimisation problem limited by geopolitical shocks.

Wu et al. [19] lay the foundation for real-time AI control of energy systems by articulating goals that minimise latency and energy per bit under hardware and protocol constraints in integrated sensing, communication, and computation. According to Letaief et al. [131], Edge AI for 6G aims to achieve energy-efficient inference at the network edge while meeting the connectivity and quality of service requirements that govern energy applications like smart grids and e-mobility. As explained by Hua et al. [126] and Wang et al. [127], photonic accelerators and co-designed chip I/O aim for ultra-low-latency, low-power AI computation under fabrication and physical constraints, allowing for more ambitious AI-IES optimisation in real time. While Fu et al. [110] employ knowledge-integrated GANs to produce weather scenarios that increase the feasible space for reliable PV integration studies, Zhang et al. [142] demonstrate how AI-accelerated platforms for emerging photovoltaics embed discovery objectives within experimental and manufacturing constraints at the materials and device layer.

### 5.5 Performance-Indicator Classification for AI-Driven Integrated Energy Systems

RMSE, MAE, MAPE,  $R^2$  and other error metrics are used to benchmark models in forecasting studies; these metrics are frequently supplemented with adversarial robustness and interpretability criteria. While a cloud-integrated framework for residential solar forecasting couple's LSTM-based prediction with end-use energy management, with a focus once more on time-series accuracy metrics, heat-load forecasting for district and regional systems explicitly combines advanced data-driven models with adversarial training to enhance robustness [106]. Neural-computation-driven emission forecasting in automotive systems [143], knowledge-integrated GANs for synthetic weather time series tailored to PV integration [110], and AutoML-based PV power prediction with SHAP interpretability [111] are all supported by similar accuracy-focused KPIs. When taken as a whole, these works establish PI-1 as the predictive baseline for any higher-layer planning, control, or optimisation logic.

Techno-economic and environmental optimisation indicators (PI-2) make up a second, equally significant cluster in Table 9, where the focus switches from pure prediction to multi-objective trade-offs between cost, efficiency, and decarbonisation. AI-enhanced techno-economic assessment optimises multi-vector coordination of energy hubs with underground storage. It benchmarks configurations that incorporate AI-based maritime scheduling in the broader energy-logistics chain using metrics like LCOE, NPC, and emission reduction [2]. Multi-objective optimisation of solar-driven hydrogen production and PEMFC-based systems assesses performance by combining economic viability, hydrogen yield, and energy efficiency across climates [45, 144]. Within AI-assisted optimisation loops, process-integration studies of biomass-driven SOFC-ammonia systems and IGFC/CCS plants use tri-objective functions involving cost, environmental performance, and efficiency [79]. Water-resource-recovery facilities and AI-optimized geothermal-desalination-hydrogen schemes use integrated economic-environmental KPIs to measure resource productivity, carbon neutrality, and circularity at the infrastructure scale [43, 17]. This cluster pushes AI beyond accuracy in order to design PtX chains and low-carbon, cost-optimal system layouts [145].

The third performance cluster, PI-3: reliability, safety, and resilience indicators, captures a smaller but strategically significant portion of the corpus by evaluating AI in terms of system risk, robustness, and fault-handling capability. Availability and risk metrics are prioritised over simple prediction errors in the reliability assessment of autonomous maritime navigation systems under uncertainty [146]. By combining reliability and lifecycle criteria, digital twin-driven health management in microgrids tracks degradation and remaining useful life at the system level using PHM-style indicators [65]. The quality of frequency regulation and resilience to disturbances are the main performance indicators in weak microgrids that use redox-flow batteries and AI-based controllers [77]. While fault and hazard metrics, which report detection rates and false alarms as core KPIs, dominate UAV-based PV fire-hazard detection using AI and SCADA streams, deep-learning power-quality assessment in grid-connected PV plants depends on classification accuracy over harmonic and distortion signatures [141]. Safety, security, and resilience are anchored as first-class performance dimensions for AI-energy integration in this cluster, along with work on neuromorphic anomaly detection and smart-grid intrusion detection [147, 98]. Computational and algorithmic efficiency (PI-4) is a separate performance layer in Table 9, which reflects the fact that edge, embedded, and high-throughput AI hardware is becoming more and more important in integrated

energy systems. Latency, throughput, and energy-per-inference metrics are used to compare large-scale photonic accelerators and co-designed silicon photonics I/O fabrics in order to assess their viability for real-time grid and energy-IoT applications [126]. Response time and energy efficiency are cited as important metrics of merit by photocapacitors and neuromorphic devices for low-light edge computing [148, 149]. Area–power–performance trade-offs are used to support the deployment of FPGA-based accelerators for neural activation and EV battery management, as well as in-memory computing units employing STT-MRAM, in constrained EV and microgrid controllers [129, 150, 130]. By evaluating spectral efficiency, latency, and scalability indicators, federated LoRaWAN architectures and SAGIN resource-management frameworks extend this computational lens to large-scale IoT and 6G environments [68, 67, 151]. This cluster shapes what is practically deployable inside energy infrastructures because AI performance is inextricably linked to hardware and network efficiency [152–157].

To create joint performance surfaces for comfort–energy co-optimisation, digital-twin-based deep-learning frameworks in buildings explicitly assess thermal comfort indices in addition to energy savings [4, 86]. Urban mobility and UAV-based logistics architectures characterise eco-efficient mobility using composite sustainability and service-quality metrics, including energy savings, routing efficiency, and emission reduction [94, 95]. Rather than using only technical KPIs, edge inference systems for visually impaired users integrate latency, accuracy, and user-assistance quality as interconnected performance dimensions [158]. At the planning scale, deep-renovation roadmaps are informed by AI-driven morphological classification of school building stock and fuzzy decision support for nature-based solutions in buildings. These processes rely on renovation potential, energy-sustainability gains, and decision-quality metrics [87, 88]. To benchmark maturity and gaps in AI–energy integration, bibliometric and systematic reviews of AI in PV, HRES, hydrogen, and battery technologies present evidence-based knowledge indicators, such as citation networks, topic coverage, and research-front mapping (Elaziz Waseef, A.A.; Kaur et al. [64]; Sai Ramesh et al. [48]).

**Table 9.** Performance-indicator classification for AI–Driven Integrated Energy Systems

| Performance-indicator cluster                | Typical metrics & evaluation focus                                                                                                                                                                                 | Dominant AI-driven functional roles in corpus                                                                                                                                                                           | Typical AI method families (indicative)                                                                                                                                | Evidence density in 153-reference corpus                                                                                                                                         | Representative topics / applications                                                                                                                                                    | Illustrative references from Table 1*                                                                                                                                            |
|----------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| PI-1: Predictive-accuracy-centred indicators | Error and fit metrics: RMSE, MAE, MAPE, MBE, $R^2$ ; classification accuracy, precision/recall, F1 score; sometimes adversarial robustness, uncertainty bounds and calibration curves for probabilistic forecasts. | Forecasting / estimation and early-warning: load and heat-demand forecasting, PV and CSP power prediction, emission and weather prediction, power-quality classification, building-stock and morphology classification, | Sequence models (LSTM/RNN), CNNs and hybrid DNNs; AutoML pipelines with tree ensembles (RF, XGBoost); GAN-based synthetic data generators; explainable ML (SHAP, XAI); | High – a large share of forecasting and estimation studies centre performance evaluation on predictive accuracy, sometimes extended with robustness and interpretability lenses. | Regional heat-load forecasting with adversarial training; multimodal power-demand forecasting; PV power output prediction with AutoML + SHAP; LSTM-driven solar forecasting in a cloud- | Zhu et al. [210]; Devanathan et al. [105]; Bakht et al. [111]; Fu et al. [110]; Zimakowska-Laskowska et al. [143]; Prakash et al. [78]; Inteha et al. [211]; Wigger et al. [120] |

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|                                                               |                                                                                                                                                                                                                                                                                                               | project-risk and charge-profile estimation.                                                                                                                                                                                                                                                                                                        | classical regression/ML for baselines.                                                                                                                                                                                                                              |                                                                                                                                                                                | integrated residential platform; emission forecasting for automotive systems; deep-learning power-quality assessment in grid-connected PV; day-ahead load forecasting and EV charge-profiling.                                                                                                                                                                                                                                                                                                                                                                        |                                                                                                                                                                                                                   |
| PI-2: Techno-economic & environmental optimisation indicators | Economic and environmental KPIs: NPC, NPV, LCOE, LCOH, total cost of ownership, payback, revenue; efficiency and exergy (%), fuel utilisation, energy savings; CO <sub>2</sub> -eq reduction, carbon-neutrality indices, circularity scores, water/energy productivity; occasionally social or policy scores. | Design, planning and multi-objective optimisation: sizing and layout of multi-vector hubs, PtX chains and H <sub>2</sub> refuelling stations; CSP and solar dryers; geothermal-desalination cycles; biomass-SOFC and IGFC/CCS plants; district-scale water-resource recovery; mega-scale industrial parks and smart-city decarbonisation pathways. | Hybrid ANN + metaheuristic optimisation (GA, PSO, NSGA-II); classical multi-objective optimisation with surrogate models; DRL-based multi-objective dispatch; techno-economic simulators coupled with ML surrogates; knowledge-guided GANs for scenario generation. | High – most design-oriented, process-integration and planning papers focus on economic–environmental trade-offs and scenario-based optimisation as primary performance lenses. | Coordinated energy management in multi-vector systems with underground storage; AI-based optimisation of PEMFC, IGFC/CCS and biomass-driven SOFC–NH <sub>3</sub> plants; techno-economic design of H <sub>2</sub> refuelling stations; geothermal cycles with integrated desalination and H <sub>2</sub> production; carbon-neutral water-sector case studies; techno-economic assessment of mega-scale industrial parks (Mega-DIP); optimisation of solar dryers and MXene-based solar fluids; multi-criteria optimisation of nano-materials for EV supercapacitors. | Taghavi et al. [2]; Assareh et al. [144]; Mansir [176]; Dou et al. [62]; Chen et al. [179]; Heo et al. [24]; Farzin et al. [17]; Li et al. [79]; Yin et al. [43]; Loksupapaiboon et al. [118]; Patil et al. [171] |
| PI-3: Reliability, safety &                                   | Reliability and quality metrics: availability, ENS,                                                                                                                                                                                                                                                           | Resilience assessment, fault detection,                                                                                                                                                                                                                                                                                                            | Digital-twin and PHM frameworks;                                                                                                                                                                                                                                    | Moderate but critical – fewer papers                                                                                                                                           | Reliability assessment of autonomous                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | Bashan [146]; Ebrahimi et al. [65]; Pajooh et                                                                                                                                                                     |

|                                                         |                                                                                                                                                                                                                                                                                                                                                                 |                                                                                                                                                                                                                                                                                                                                                |                                                                                                                                                                                                                  |                                                                                                                                                                                                        |                                                                                                                                                                                                                                                                                                                                                                                         |                                                                                                                                                                                                                                                           |
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| resilience indicators                                   | LOLP; fault- and hazard-detection rates, confusion-matrix metrics, false-alarm and missed-detection rates; power-quality indices (THD, voltage/frequency deviation); resilience proxies such as downtime, recovery time, robustness under uncertainty; PHM indicators for component and system health.                                                          | security and lifecycle PHM: frequency regulation in weak microgrids; reliability assessment for autonomous or maritime systems; digital-twin-driven health management; smart-grid intrusion and anomaly detection; fire-hazard detection in PV plants; PHM for marine hybrid systems; power-quality assessment and magnetic-anomaly detection. | anomaly-detection DNNs and CNNs (including UAV-image analysis); hybrid ML–signal-processing for PQ assessment; RL/DRL for resilient control; expert/fuzzy systems for detection and risk scoring.                | than PI-1/PI-2, but these indicators are pivotal for high-reliability AI–IES deployment and for bridging safety cases with AI control.                                                                 | maritime navigation under uncertainty; digital twin-driven health management in microgrids; redox-flow-battery frequency regulation in weak microgrids; smart-grid intrusion detection; UAV-assisted PV fire-hazard detection; PHM for marine hybrid energy systems; deep-learning-based power-quality assessment; neuromorphic and nanodevice-assisted anomaly detection.              | al. [77]; Lysyi et al. [141]; Abou-Elasaad et al. [98]; Tang et al. [51]; Prassanth et al. [59]; Prakash et al. [78]; Qin et al. [147]                                                                                                                    |
| PI-4: Computational & algorithmic efficiency indicators | Algorithmic and system-level efficiency: inference latency, end-to-end response time, throughput (GFLOPS/TOPS), computational complexity, scalability with problem size, memory footprint, power and energy per inference; area–power–performance trade-offs on FPGA/ASIC/photonic platforms; network-level efficiency (spectral efficiency, link utilisation). | Enabling real-time and embedded AI: timing-guaranteed embedded inference; edge AI and federated learning in IoT/LoRaWAN; AI accelerators for EV battery management and smart-grid analytics; photonic and in-memory computing for petascale connectivity; hardware-aware AI deployment in SAGIN and 6G networks.                               | Hardware-aware DNNs; FPGA and ASIC accelerators; photonic neural accelerators; in-memory computing with STT-MRAM; model-compression and quantisation; edge/federated learning protocols for constrained devices. | High among ICT/hardware-focused works – a substantial subset of the corpus is devoted to AI acceleration, edge-AI timing guarantees and scalable connectivity, forming the digital backbone of AI–IES. | Integrated large-scale photonic accelerators with ultra-low latency; co-designed silicon photonics chip I/O for energy-efficient petascale connectivity; photocapacitors for low-light edge computing; FPGA-based accelerators for EV battery management and neural activation; STT-MRAM in-memory computing units; MDAC-less ADCs for medical-imaging AI; resource-efficient federated | Hua et al. [126]; Wang et al. [79]; Flores-Díaz et al. [148]; Hingu et al. [129]; Nagarale et al. [150]; Saha et al. [130]; Triantafyllou et al. [68]; Jia et al. [209]; Mahboob et al. [151]; Behera et al. [212]; Zhao et al. [209]; Akabe et al. [213] |

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|                                                                      |                                                                                                                                                                                                                                                                                                                                                                                                                      |                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |                                                                                                                                                                                                                                                          |                                                                                                                                                                                                              | LoRaWAN architectures; SAGIN access networks with pervasive intelligence; 6G-ready O-RAN, metasurface antennas and energy-harvesting nonvolatile processors.                                                                                                                                                                                                                                                                                                                                                                                                                           |                                                                                                                                                                                                                                     |
| PI-5: Multi-criteria comfort, service-quality & synthesis indicators | Composite indices: thermal comfort (PMV/PPD, adaptive comfort indices), indoor air-quality and comfort–energy trade-off scores; QoS and QoE (latency, accessibility, reliability) for mobility, logistics and assistive systems; sustainability and resilience scores; for reviews/bibliometric s: citation counts, co-citation and keyword-co-occurrence networks, thematic coverage and research-front indicators. | Building operations, urban mobility, assistive systems and knowledge synthesis: personalised thermal comfort and energy-efficient building operation; carbon-neutral smart buildings; eco-efficient urban logistics and UAV-enabled delivery; assistive navigation for visually impaired users; nature-based and morphology-based decision support for building projects; policy-oriented and bibliometric syntheses of AI in PV, HRES, hydrogen and batteries. | Deep learning and digital-twin frameworks; hybrid control for comfort–energy optimisation; fuzzy-MCDM and rule-based decision support; generative and spatial AI for urban twins; bibliometric analysis pipelines with clustering and network analytics. | Moderate–High – when bibliometric and review studies are included, a significant fraction of the corpus reports multi-criteria comfort, service or knowledge-synthesis indicators alongside energy and cost. | Digital twin-based deep-learning frameworks for personalised thermal comfort and smart-building operation; AI-optimised energy and comfort control in tropical buildings; IoT architectures for sustainable urban mobility; eco-efficient UAV design for urban logistics; edge-AI assistance systems for visually impaired individuals; fuzzy decision-support for nature-based solutions in building sustainability; AI-driven morphological classification of school building stock for renovation roadmaps; data-driven policy frameworks for PV deployment and hybrid RES reviews. | Almadhor et al. [4]; Kim et al. [214]; Reis et al. [94]; Bibbò et al. [95]; Măgurean & Besoiu [158]; Bressane et al. [88]; Caccia et al. [87]; Freitas et al. [168]; Elaziz Waseef, A.A.; Kaur et al. [200]; Sai Ramesh et al. [48] |

## 6. Comparative Analysis of AI-Driven Integrated Energy Systems Typologies and Optimization Strategies

The methodological basis for categorising AI-Driven Integrated Energy Systems (AI-IES) was established in Section 6. This section expands on that framework by contrasting the main types of integrated energy systems and the optimisation techniques applied to incorporate AI into them. Three dimensions form the framework of the analysis: (i) vector couplings and system typology; (ii) dominant AI and optimisation paradigms; and (iii) decision layers and performance goals. A conceptual taxonomy description that can direct future analytical and design work is presented after a classification matrix (Table 10).

**Table 10.** Typologies of AI-Driven Integrated Energy Systems

| Typology of AI-Driven Integrated Energy System          | System boundary & coupled vectors                                                                                                                                                                                                                                                        | Dominant AI roles in the typology                                                                                                                                                                                                                          | Typical AI / data architectures                                                                                                                                                                                                                                           | Example integrated technologies & assets                                                                                                                                                                                                                    | Representative studies                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          | Key insights, trade-offs & research gaps                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
|---------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 1. Building - and district-scale multi-energy hubs      | Building, campus or district hubs coupling electricity, space heating/cooling and sometimes gas through combinations of PV, CHP, heat pumps, thermal storage, smart envelopes and ventilation. Multi-energy interaction occurs at sub-hourly timescales driven by weather and occupancy. | Predictive control of HVAC and CHP, co-optimisation of comfort and energy cost, anomaly detection, retrofit decision-support and asset sizing. AI also supports life-cycle planning by linking design choices to long-term energy and carbon trajectories. | Building and district digital twins with embedded machine-learning surrogates; deep learning-based comfort and load models; fuzzy and rule-based decision systems; ontology-enabled knowledge graphs for operation and maintenance; IoT/edge analytics for local control. | BIPV façades and rooftop PV arrays; variable-speed heat pumps; TES tanks and phase-change materials; CHP units; advanced envelopes and nature-based elements such as green roofs and façades; dense sensor networks for occupancy, comfort and air quality. | Almadhor et al. [115] use residential digital twins and statistical ML to optimise energy use and comfort in dwellings; Almadhor et al. [115] further implement deep learning for personalised thermal comfort in smart buildings; Kim et al. [86] deploy AI-optimised control for carbon-neutral tropical buildings; Yoon & Song [86] introduce ontology-enabled AI agents for building O&M digital twins; Bressane et al. [88] employ fuzzy decision support to integrate nature-based solutions into building energy planning; Mohamed et al. [140] apply ANN-based intelligent energy management across smart building portfolios; Elaziz Waseef (A.A.) provides a bibliometric perspective on PV integration in buildings. | Evidence shows that AI-driven multi-energy hubs can reconcile comfort, cost and carbon objectives when thermal and electrical vectors are co-optimised instead of managed in silos [4] [4]. District-scale digital twins begin to act as coordination fabrics across heterogeneous buildings, although model interoperability and standardised ontologies remain open challenges [86]. Studies on nature-based designs and BIPV indicate that physical design and AI control need to be co-designed rather than sequentially optimised [88]. Gaps persist around cyber-security, privacy, and robust adaptation to climate-induced extremes in district-scale hubs [86]. |
| 2. Multi-energy microgrids and community energy systems | Campus, island, rural and urban community microgrids that integrate rooftop and ground-mounted PV, small wind turbines, BESS, EV fleets, diesel or gas gensets and sometimes hydrogen storage or fuel cells. Operation spans grid-connected                                              | Multi-objective energy management (cost, reliability, emissions), real-time scheduling, frequency and voltage regulation, EV and V2G coordination, intelligent protection and resilience                                                                   | Hybrid controllers combining reinforcement learning with rule-based logic; probabilistic forecasting and optimisation; ANN-based supervisory controllers; digital twin-assisted microgrid                                                                                 | PV-battery-diesel and PV-wind-battery topologies; redox-flow and Li-ion storage; EV charging hubs with V2G; electrolyser and H <sub>2</sub> storage for seasonal shifting;                                                                                  | Khosravi et al. [18] develop AI-driven hybrid control for hydrogen-integrated microgrids with V2G; Banihabib et al. [160] optimise micro gas turbine operation in a natural gas-hydrogen microgrid using AI; Pajoo et al. [77] design AI-based controllers for redox-flow batteries providing frequency regulation in weak microgrids; Ullah et al. [52] propose an adaptive control scheme for a micro-grid with dual active bridge and battery storage; Oukhouya Ali &                                                                                                                                                                                                                                                        | Across case studies, AI improves resilience and power quality while enabling higher renewable penetration, particularly when controllers explicitly account for uncertainty and multi-carrier dynamics [18]. Hydrogen and redox-flow batteries appear as promising long-duration complements to Li-ion storage, but require richer degradation and lifetime models in community-scale optimisation [77]. Microgrid papers increasingly highlight                                                                                                                                                                                                                         |

|                                                       |                                                                                                                                                                                                                                                                                     |                                                                                                                                                                                                                                                                                                    |                                                                                                                                                                                                                                                                                             |                                                                                                                                                                                                                                                                                            |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |
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|                                                       | and islanded modes with strong stochasticity from renewables and demand.                                                                                                                                                                                                            | under contingencies. AI also supports predictive maintenance and state estimation.                                                                                                                                                                                                                 | simulators; IoT-enabled edge control for fast response.                                                                                                                                                                                                                                     | micro gas turbines embedded in microgrids; smart inverters with advanced grid-support functions.                                                                                                                                                                                           | Jamila [215] study PV- and BESS-enhanced EV charging stations with neural-network energy management; Sarker et al. [90] present an AI optimisation framework for smart EV charging integrated with PV and BESS in high-density residential settings; Almihat & Munda [133] review microgrid integration challenges for renewables.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         | social and regulatory constraints, showing that technically optimal schedules may clash with tariff design and protection standards [160]. Future work needs harmonised benchmarks and open microgrid datasets to compare AI controllers across climates and grid codes [133].                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |
| 3. Regional and national multi-vector infrastructures | Country- or region-scale infrastructures where electricity, gas, district heating/cooling and emerging hydrogen networks interact with transport and communication systems. Time horizons span day-ahead dispatch to long-term planning under geopolitical and climate uncertainty. | Long-term capacity expansion planning, cross-vector economic dispatch, congestion and security management, regional heat-load forecasting, risk assessment for energy security and decarbonisation pathways. AI also supports scenario generation and policy stress-testing.                       | Deep reinforcement learning for virtual power plants and multi-vector dispatch; surrogate models for power, gas and heat networks; large-scale time-series forecasting for heat, electricity and mobility demand; AI-enabled 6G and SAGIN communication backbones for real-time monitoring. | Integrated electricity and gas systems with underground storage; district heating and cooling networks; cross-border transmission corridors; hydrogen backbones and import/export terminals; maritime logistics linked to energy hubs; wide-area sensing and communication infrastructure. | Taghavi et al. [2] conduct techno-economic assessment of coordinated multi-vector energy management with underground storage and AI-based maritime scheduling; Tang & Wang [112] apply deep reinforcement learning to optimise virtual power plants and smart grids for renewable integration and grid efficiency; Soleimani et al. [63] review hybrid energy systems integrating heat pumps and district heating; Zhu et al. [106] advance regional heat-load forecasting with data-driven methods and adversarial training; Salman [102] analyses AI-driven energy systems within Germany's gas-exit security strategy; Saafi et al. [136] and Akgül et al. [66] describe AI-enabled 6G and B5G architectures underpinning sustainable networking for multi-vector systems; Ramos et al. [82] and Farzin et al. [17] explore water sector infrastructures as net-zero multi-vector hubs. | Large-scale studies show that AI can unlock latent flexibility across carriers, for instance by coordinating storage, maritime logistics and sector coupling to reduce system costs while preserving security of supply [2]. However, computational complexity and data fragmentation across operators limit deployment of fully integrated AI planners at national scale [112]. Emerging work on AI-enabled 6G and SAGIN networks highlights that communication reliability and cyber-security become as critical as physical redundancy for multi-vector resilience [66]. Research gaps include transparent AI methods suitable for regulatory scrutiny and integration of climate-stress scenarios, such as protracted heatwaves or gas embargoes, into multi-vector optimisation [102]. |
| 4. Sector-coupled industrial and power-to-X clusters  | Industrial parks, refinery and petrochemical zones, ports and energy-intensive clusters where electricity is converted to hydrogen, heat, fuels and chemicals (power-to-H <sub>2</sub> , -NH <sub>3</sub> , -DME, -liquids) co-located with large process loads and sometimes CCS.  | Process design and tri-objective optimisation (cost, efficiency, emissions), dynamic operation of electrolyzers and SOFCs, co-optimisation of co-products (e.g., oxygen, heat), techno-economic assessment under volatile electricity prices and policy constraints, and predictive maintenance of | Hybrid process simulators with ML-based surrogates; metaheuristic and evolutionary optimisation augmented by AI; AI-assisted digital twins of electrolysis and chemical plants; generative AI for scenario exploration and siting; advanced MPC informed by learned system dynamics.        | Solar-driven electrolyzers; biomass-driven SOFC ammonia plants; geothermal-electricity-coupled H <sub>2</sub> production and liquefaction; industrial parks using large-scale renewable and waste-heat integration; biogas and wastewater-to-energy resource recovery facilities;          | Assareh et al. [144] implement AI-based multi-objective optimisation of a solar-driven hydrogen system with integrated oxygen and power co-generation; Dou et al. [62] design a biomass-driven SOFC plant co-producing electricity and ammonia using ML-assisted tri-objective optimisation; Yin et al. [43] couple a sustainable geothermal scheme with desalinated water-based H <sub>2</sub> production and liquefaction using AI-aided optimisation; Heo et al. [24] explore generative AI-driven techno-economic and environmental assessment for a mega-scale decarbonised industrial park; Farzin et al. [17] apply an AI optimisation framework to biogas-based energy circularity in water resource recovery facilities;                                                                                                                                                          | Sector-coupled clusters appear as crucial laboratories where AI coordinates electrochemical, thermal and chemical subsystems, revealing deep decarbonisation pathways that conventional heuristics would miss [144]. Many studies show that AI-enhanced process optimisation can shift systems from marginal efficiency gains to step-changes in carbon intensity when combined with CCS and circular resource use [62]. Yet, water use, land constraints and infrastructure lock-in remain under-represented in current optimisation formulations [43]. There is also a need for robust, open digital twins of industrial clusters that                                                                                                                                                    |

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|                                                     |                                                                                                                                                                                                                                                                               | critical process units.                                                                                                                                                                                                                                                                                         |                                                                                                                                                                                                                                                                                                                | renewables-powered desalination and hydrogen production.                                                                                                                                                                                                                                  | Chekifi et al. [84] discuss AI opportunities in renewables-powered desalination; Christopher Selvam et al. [164] and Wei et al. [81] examine AI applications across hydrogen production and storage chains; Zamora-Aguirre et al. [80] optimise integrated green dimethyl ether production with AI.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | integrate market volatility, policy risk and multi-vector physical constraints into a unified AI planning environment [24].                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
| 5. Urban energy twins and platform-based ecosystems | City- and district-scale systems where AI-enabled digital twins integrate electricity, heat, mobility, and sometimes water, waste and green infrastructure. Scope spans buildings, transport, distributed generation, public lighting, water treatment and urban agriculture. | System-of-systems coordination, urban planning and zoning support, mobility and charging optimisation, distributed generation placement, multi-sector demand response, and policy analytics for emissions, equity and resilience. AI also underpins citizen-facing services and participatory decision-support. | Generative spatial AI for urban digital twins; IoT-centred data fabrics with edge and cloud analytics; multi-agent reinforcement learning for mobility and energy; federated learning across districts; integrated sensing-communication-computation stacks (5G/6G, LoRaWAN, SAGIN) for dense urban telemetry. | City-wide BIPV and rooftop PV portfolios; EV fleets and charging corridors; district heating and cooling; urban wind and roadside PV; smart street lighting; water and wastewater treatment plants; smart irrigation and green infrastructure; sensorised public transport and logistics. | Yoon & Song [166] present ontology-enabled AI agents for building digital twins that form modular components of wider urban twins; Huang et al. [89] propose generative spatial AI for sustainable smart cities via large-flow urban digital-twin models; Reis et al. [94] design an IoT architecture for energy-aware, low-emission urban mobility; Ning [167] develops AI-driven decision support for sustainable energy management in smart cities; El-Barbary et al. [96] implement an AI-driven IoT framework for wind-energy monitoring in smart-city contexts; Banluesapy et al. [122] apply AI-augmented smart irrigation using IoT and solar power, linking water and energy in peri-urban landscapes; Freitas et al. [168] use AI to accelerate data-driven PV policy in Lisbon; Wu et al. [19] survey AI-enabled integrated sensing, communication and computation; Triantafyllou et al. [68] propose resource-efficient federated LoRaWAN for far-edge IoT in cities. | Urban energy twins and platforms reframe cities as learning systems where physical and digital infrastructures co-evolve, enabling joint optimisation of energy, mobility and environmental quality [89]. Empirical studies highlight substantial gains in PV adoption, mobility emissions and water-energy nexus efficiency when AI analytics and IoT architectures are integrated into planning and operations [94, 122]. Nonetheless, governance, data equity and cyber-security become central constraints, as critical infrastructures and personal data converge within unified platforms [168]. Future research needs co-designed regulatory sandboxes, open data standards and human-centric design of AI services to ensure that urban energy twins advance just and inclusive energy transitions [167]. |

## 6.1 Typologies of AI-Driven Integrated Energy Systems

### 6.1.1 Building- and District-Scale Multi-Energy Hubs

Almadhor et al. [4] show how statistical machine learning and residential digital twins can work together to optimise HVAC schedules and on-site generation while capturing intricate building physics and occupant behaviour. Almadhor et al. [4] also show that, as shown in Fig. 16, AI-driven multi-energy hubs are characterised by individualised thermal comfort under strict energy-efficiency constraints, made possible by deep learning-based comfort models integrated into building control loops. This logic is extended by Kim et al. [86] to carbon-neutral tropical buildings, where AI-optimised energy and comfort control integrates passive measures, active cooling, and photovoltaic systems to manage indoor comfort and decarbonisation goals. In intelligent building digital twins, Yoon and Song [86] present ontology-enabled AI agents that enable semantics-aware operation and maintenance of the HVAC, electrical, and heating subsystems. Bressane et al. [88] demonstrate how AI can integrate green infrastructure,

thermal performance, and energy use within a single district-scale decision framework by evaluating nature-based solutions for building projects at the design and planning level using a fuzzy-based decision-support system. To demonstrate how multi-energy hubs develop into learning systems that continuously adjust to load, weather, and user patterns, Mohamed et al. [140] supplement these efforts with an Internet of Things (IoT)-driven intelligent energy management system that employs artificial neural networks for smart monitoring and control in building portfolios [159].

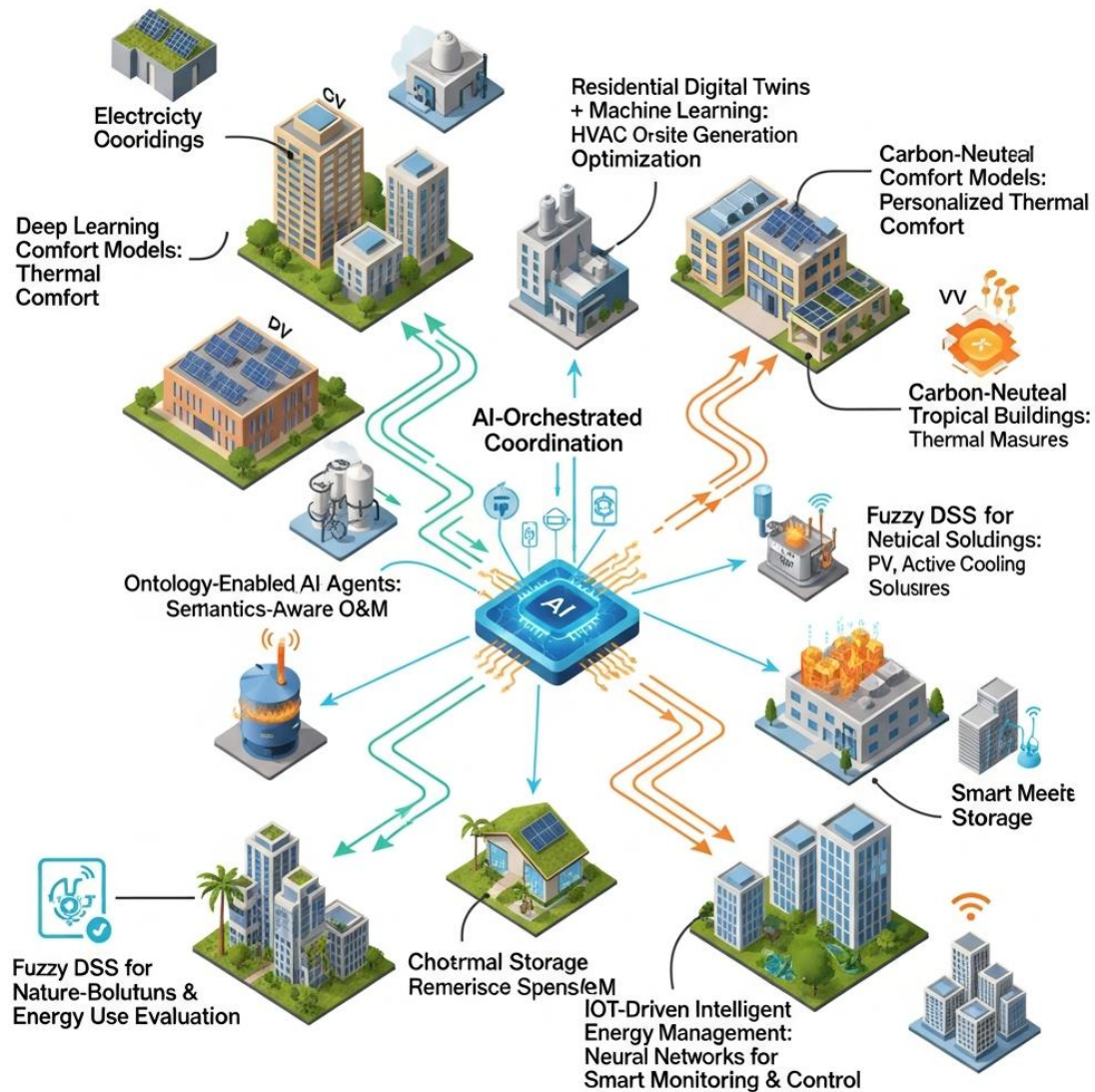


**Fig. 16.** Typologies of AI-Driven Integrated Energy Systems utilising Building- and district-scale multi-energy hubs

### 6.1.2 Multi-energy Microgrids and Community Energy Systems

Khosravi et al. [18] use probabilistic energy management to balance stochastic renewable generation, EV charging, and reliability constraints in their AI-driven hybrid control scheme for hydrogen-integrated microgrids with vehicle-to-grid (V2G)

participation. In a microgrid running on natural gas and hydrogen, Banihabib et al. [160] use AI-based optimisation to reduce operating costs and emissions while preserving power quality. Redox flow batteries in weak microgrids, where AI-based controllers provide reliable frequency regulation under high renewable penetrations, are the subject of Pajoo et al. [77]. To demonstrate how AI-enhanced control strategies stabilise multi-energy community systems under rapidly shifting load and generation profiles, Ullah et al. [52] provide an industrial-grade adaptive control scheme for a microgrid with a dual active bridge and battery storage. Oukhouya Ali and Jamila [43] combine classical optimisation and neural network solutions to suggest energy management strategies for PV and battery storage-enhanced EV charging stations at the nexus of microgrids and e-mobility. While Almihat and Munda [133] synthesise integration challenges for renewable energy in microgrids, highlighting interoperability, protection, and coordination issues that AI-based controllers are starting to address, Sarker et al. [90] add a high-density residential perspective by implementing an AI-driven optimisation framework for smart EV charging integrated with rooftop PV and BESS [161].

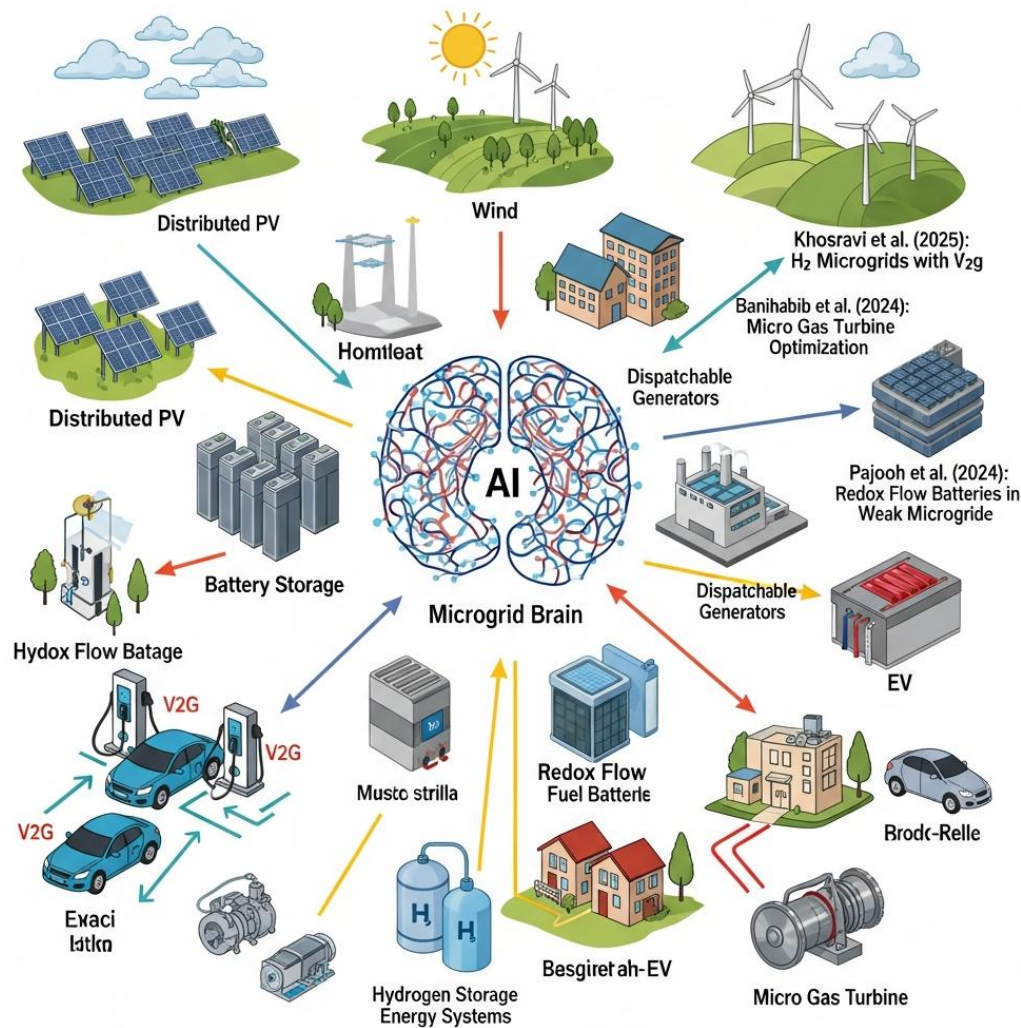


**Fig. 17.** Typologies of AI-Driven Integrated Energy Systems utilising Multi-energy microgrids and community energy systems

### 6.1.3 Regional and National Multi-Vector Infrastructures

The integration concept is extended to coupled electricity, gas, district heating/cooling, and emerging hydrogen networks by regional and national multi-vector infrastructures in the corpus, frequently for market and security constraints. As illustrated in Fig. 18, Taghavi et al. [2] present a techno-economic assessment framework for coordinated energy management in multi-vector systems, utilising AI-based maritime scheduling and subterranean storage to lower system-wide costs while adhering to cross-vector capacity limits. Tang and Wang [112] apply deep reinforcement learning to virtual power plants and smart grids, treating grid efficiency and renewable integration as shared goals constrained by network dependability and power-flow viability over large areas. In their review of hybrid energy systems that combine district heating and heat pumps, Soleimani et al. [63] describe how AI-enabled modelling enables coordinated dispatch across thermal and electrical networks. By utilising advanced data-driven techniques and adversarial training, Zhu et al. [106] improve regional heat-load forecasting, which serves as the predictive foundation for resilient district heating control in the face of climate variability. To manage supply security and decarbonisation at the same time, energy policy interacts with AI-enabled infrastructures, as shown in Salman's (2025) analysis of Germany's energy security strategy during the Russian gas exit. Akgül et al. [66] present a sustainable 6G architecture, while Saafi et al. [136] investigate AI-aided integrated terrestrial and non-terrestrial 6G solutions for maritime networking [162, 163].

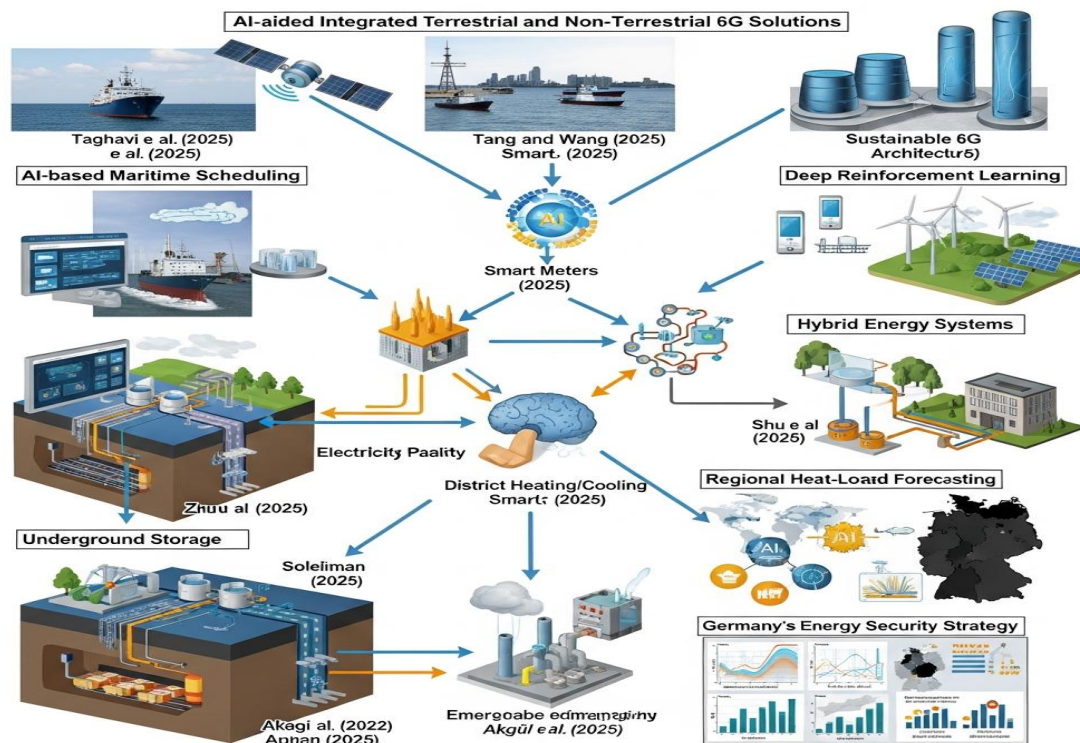


**Fig. 18.** Typologies of AI-Driven Integrated Energy Systems utilising Regional and national multi-vector infrastructures

#### 6.1.4 Sector-Coupled Industrial and Power-To-X Clusters

Assareh et al. [144] propose a multi-objective optimisation of a solar-driven system for hydrogen production with integrated oxygen and power co-generation. AI-based machine learning facilitates the tri-objective optimisation of efficiency, cost, and environmental performance in Dou et al.'s (2025) simulation of a biomass-driven SOFC plant that uses green hydrogen to produce electricity and ammonia. Yin et al. [43] use AI-assisted optimisation to manage intricate thermodynamic and financial trade-offs in their sustainable geothermal scheme, which combines cooling and power cycles with desalinated water-based hydrogen production and liquefaction. According to Heo et al. [24], generative AI powers techno-economic and environmental evaluations of renewable and sustainable energy use in mega-scale decarbonised industrial parks in the petrochemical industry, thereby establishing integrated power-to-X clusters. By redefining wastewater plants as energy-circular hubs, Farzin et al. [17] present an AI-driven optimisation framework for biogas production in water resource recovery facilities. Wei et al. [81] review AI applications in hydrogen systems, Christopher Selvam et al. [164] survey progress in water electrolysis and storage for green hydrogen, and Chekifi et al. [84] highlight desalination powered by renewables as both a challenge and an AI opportunity. Together, these studies demonstrate how AI supports design and operation across industrial power-to-X chains [165].

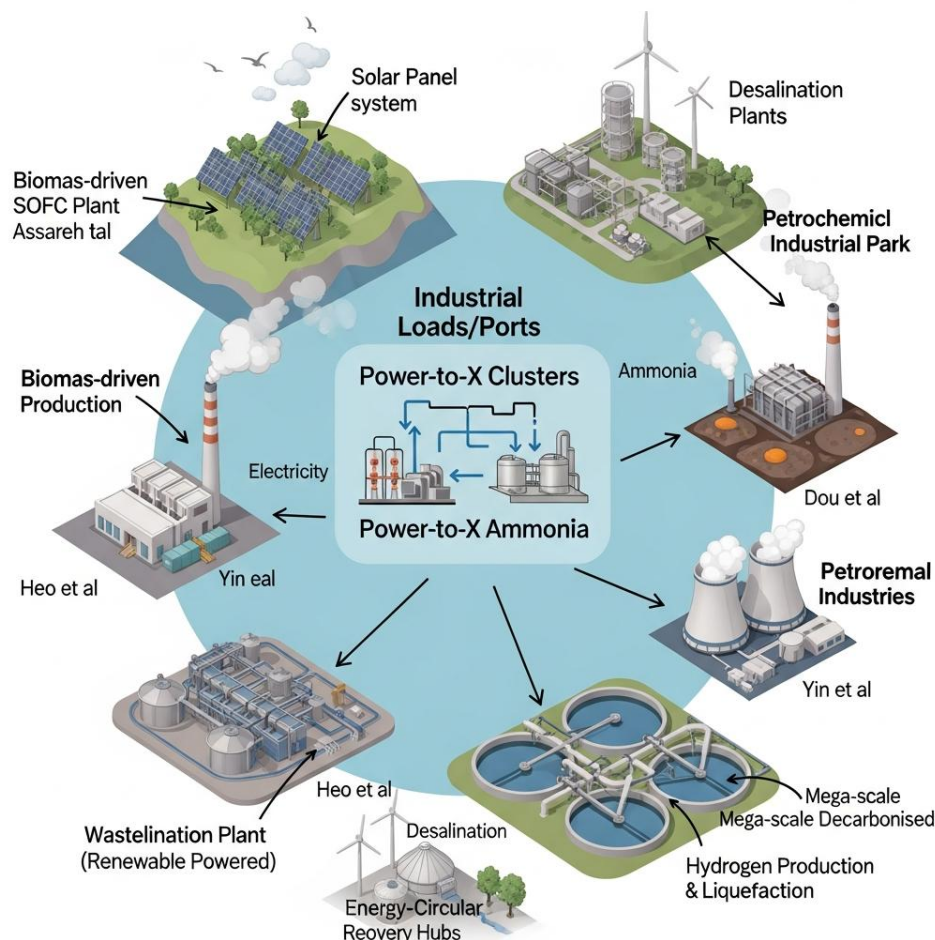


**Fig. 19.** Typologies of AI-Driven Integrated Energy Systems utilising Sector-coupled industrial and power-to-X clusters

### 6.1.5 Urban Energy Twins and Platform-Based Ecosystems

As illustrated in Fig. 20, urban energy twins and platform-based ecosystems represent an emerging typology in which artificial intelligence (AI) is integrated into digital representations of cities or districts, capturing the flows of heat, electricity, mobility, and occasionally water and waste. Yoon and Song [166] describe ontology-enabled AI agent-driven digital twins for building operations and maintenance. In their proposal for a generative spatial AI framework for sustainable smart cities, Huang et al. [89] use a large-flow model for urban digital twins that can encode land-use patterns, mobility networks, and energy infrastructures in a single computational environment. Energy-aware and low-emission smart cities are the focus of Reis et al.'s (2025) IoT architecture for sustainable urban mobility, which demonstrates how AI-based analytics on charging and mobility data interact with urban electricity systems. Ning [167] highlights cross-domain optimisation across lighting, buildings, and transportation while introducing AI-driven decision-support systems for sustainable energy management in smart cities. While Banluesapy et al. [122] demonstrate how AI-augmented smart irrigation utilising IoT and solar power connects water and energy management in peri-urban and agricultural interfaces, El-Barbary et al. [96] offer an AI-driven IoT framework for wind energy monitoring and performance enhancement in smart cities. Wu et al. [19] discuss AI-enabled integrated sensing, communication, and computation, defining the digital infrastructure required to support such platform ecosystems, while Freitas et al. [168] add a policy and governance dimension by showcasing an AI-based framework to speed data-driven policies for solar PV adoption in Lisbon. With the help of these studies, planners, operators, and policymakers can co-optimize multi-vector energy flows, mobility, and environmental quality in a closely connected, data-rich urban fabric by using urban energy twins, which are living, AI-driven platforms.

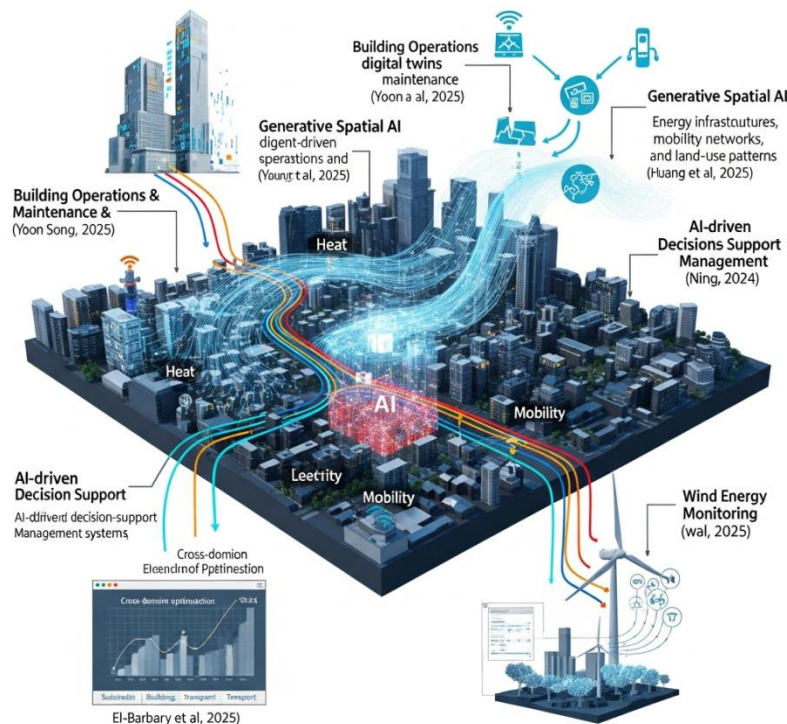


**Fig. 20.** Typologies of AI-Driven Integrated Energy Systems utilising Urban energy twins and platform-based ecosystems

## 6.2 Optimization and Control Strategies across Typologies

### 6.2.1 Deterministic Mathematical Programming

Since it can encode intricate physics, equipment limitations, and market rules within mixed-integer or nonlinear formulations, deterministic mathematical programming continues to be the mainstay for long-term sizing and expansion planning across multi-energy hubs, microgrids, and regional multi-vector infrastructures (Fig. 21). With hourly or sub-hourly resolution, typical MILP and MINLP models co-optimize investment and operation over horizons ranging from one to twenty years. They frequently involve thousands of binary variables for on/off states, unit commitment, and network expansion decisions in coupled electricity–heat–gas–hydrogen architectures. Deterministic formulations can minimise net present cost, CO<sub>2</sub> emissions, and curtailed energy while adhering to shipping schedules and storage limits in coastal hubs and ports, as demonstrated by techno-economic evaluations of coordinated multi-vector systems with underground storage and AI-based maritime scheduling [2]. Deterministic capacity-expansion models are the most widely used method for assessing district-scale hubs and their interactions with multi-energy networks, according to systematic reviews of hybrid renewable energy systems that combine district heating and heat pumps [63]. Fuel cell stack sizes, capture units, and balance-of-plant are co-optimised subject to thermal integration and carbon intensity constraints in the techno-economic optimisation of IGFC/CCS systems based on synergistic energy gradient utilisation, which is supported by similar formulations [79]. Deterministic optimisation generally yields double-digit reductions in levelised cost and emissions compared to heuristic baselines for hydrogen refuelling stations, building-integrated photovoltaic systems, and hybrid hydrogen systems while maintaining strict feasibility with regard to comfort, reliability, and environmental constraints [14, 64, 169].

### 6.2.2 Stochastic and Robust Optimisation

By directly incorporating uncertainty in renewables, demand, and prices into the optimisation process—usually through scenario trees, chance constraints, or distributionally robust formulations—stochastic and robust optimisation expand on this foundation. As illustrated in Fig. 22, GAN-enhanced robust optimisation in grid-integrated PV systems explicitly perturbs year-round weather and irradiance time series to generate ensembles of plausible trajectories, resulting in inverter and feeder settings that are still feasible under extreme ramps and forecast errors while limiting worst-case losses of PV hosting capacity [23]. Stochastic representations of wind, PV, load, and hydrogen demand are introduced in probabilistic energy management frameworks for hydrogen-integrated microgrids. Battery, electrolyser, fuel cell, and vehicle-to-grid schedules are co-optimized to minimise expected operating costs, subject to reliability metrics like conditional value-at-risk of unserved energy and loss of load probability [18]. Similar to this, tri-objective optimisations of biomass-driven SOFC-based electricity and ammonia plants treat feedstock availability, price, and electricity tariffs as stochastic drivers. They also explore large Pareto sets that balance cost, CO<sub>2</sub> emissions, and energy efficiency under multi-scenario operation [62]. AI-aided optimisation uses market models and stochastic thermodynamics to quantify how reservoir performance and hydrogen price uncertainty affect optimal sizing and dispatch decisions in geothermal, desalination, and hydrogen schemes. This reveals trade-offs between nominal cost and robustness in multi-vector regional systems [43]. As demonstrated by AI-driven optimisation in water resource recovery facilities, where the objective is to maintain carbon neutrality across

variable inflows and biogas yields, these stochastic and robust approaches are becoming more and more integrated into sector-coupled water, hydrogen, and bioenergy infrastructures [17].



**Fig. 21.** Optimization and control solutions across typologies utilizing deterministic mathematical programming

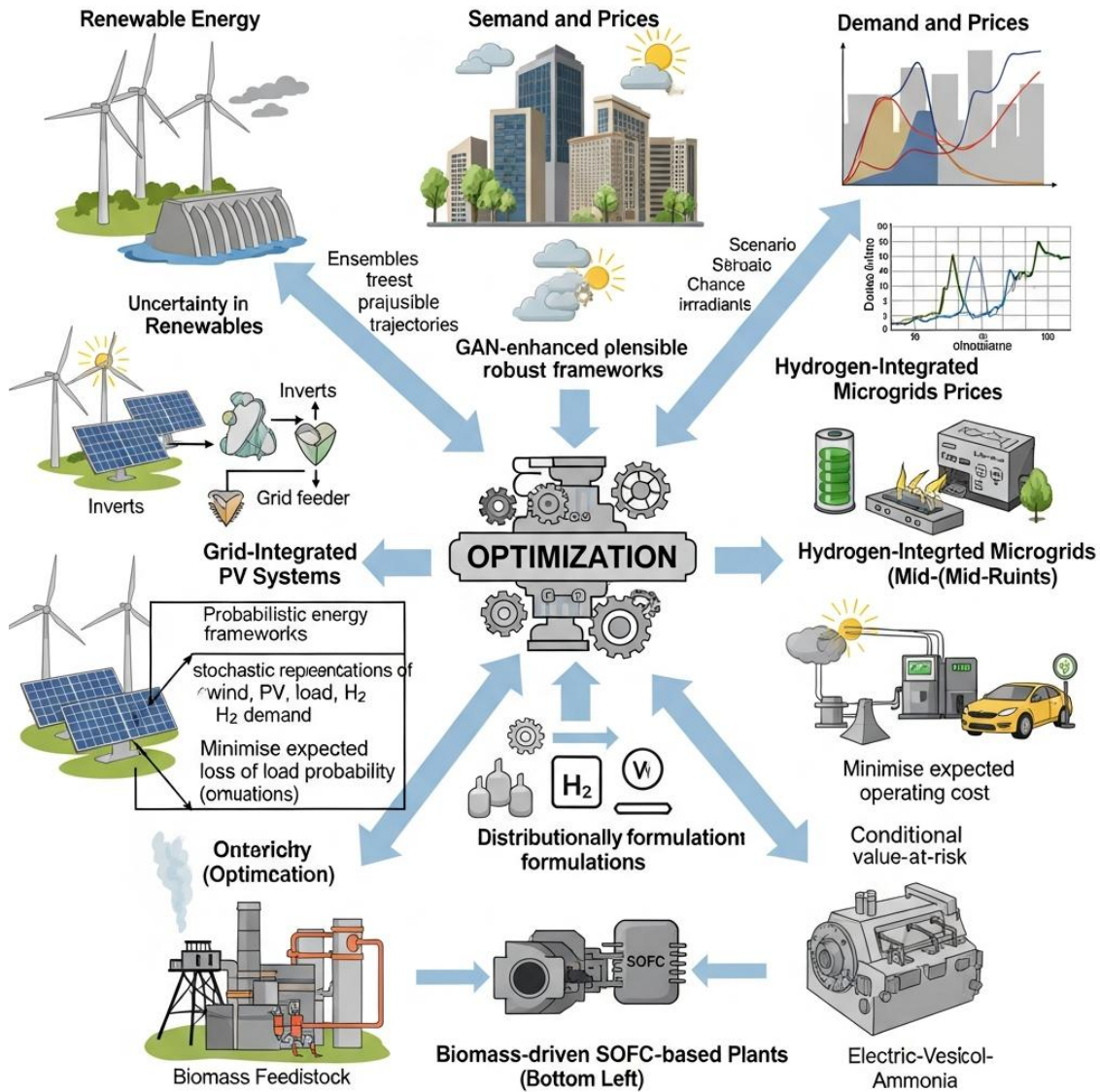


**Fig. 22.** Optimization and control solutions across typologies utilising Stochastic and robust optimisation

### 6.2.3 Metaheuristics and Evolutionary Optimisation

For highly non-convex, black-box, and multi-objective design problems that defy classical convex programming, especially in component-level and process-intensive IES studies, metaheuristics and evolutionary optimisation offer a supplementary toolkit (Fig. 23). By employing surrogate models rather than costly CFD simulations, AI-driven modelling and metaheuristic optimisation of PEM fuel cells show how genetic algorithms and differential evolution can simultaneously tune geometric, operating, and material parameters to maximise power density and durability while minimising voltage losses [45]. Advanced PV module designs can be adjusted across parameter spaces with hundreds of design variables at the building and device scale through numerical modelling using neural-network surrogates and particle swarm optimisation, exploring Pareto fronts spanning cost, thermal management, and electrical efficiency [60]. Solar dryers, CSP plants, and green fuel production chains are increasingly using metaheuristic

hybrids, like ANN–GA frameworks, where CFD or process simulators are disguised as black-box evaluators and GA/PSO populations of 50–200 people navigate discrete design choices (collector geometries, storage sizes, operating temperatures) across thousands of evaluations to find effective configurations [118, 170, 80]. Multi-criteria metaheuristic optimisation of nano-material supercapacitors and MXene-based ionic liquids in transport and storage typologies captures high-dimensional trade-offs between energy density, cycle life, safety, and sustainability, bringing component-level designs into line with system-level requirements for solar thermal plants and electric vehicles [171, 46]. When combined, these evolutionary techniques allow for the investigation of expansive, irregular design areas in sector-coupled industrial clusters, microgrids, and building-scale hubs where classical gradients are either unreliable or unavailable [92].

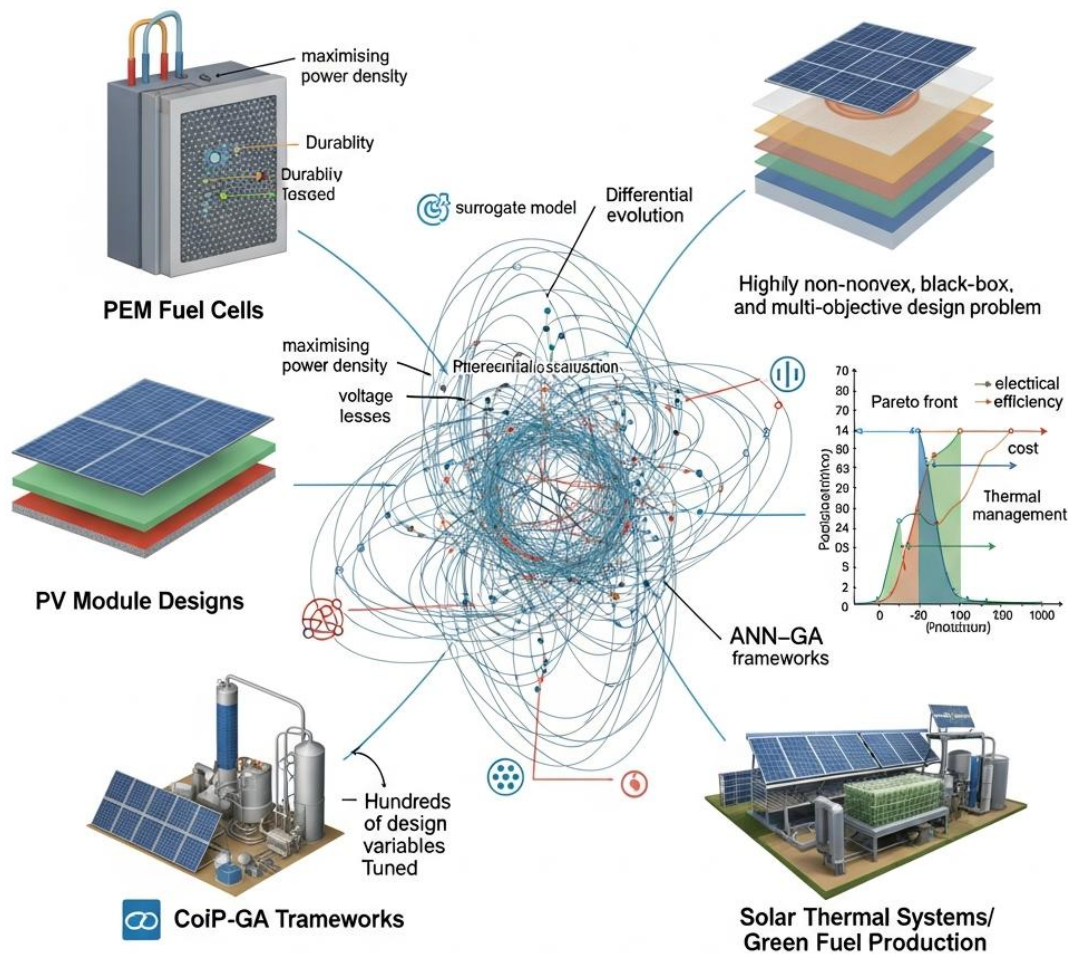


**Fig. 23.** Optimisation and control solutions across typologies utilizing Metaheuristics and evolutionary optimization

#### 6.2.4 Learning-Based Control and Coordination

Learning-based control and coordination, which is frequently applied on top of deterministic or metaheuristic planning, closes the loop by integrating reinforcement learning, multi-agent reinforcement learning, and AI-enhanced MPC into the day-ahead and real-time operation of integrated energy systems, as illustrated in Fig. 24. In

thousands of simulated episodes, deep reinforcement learning frameworks for virtual power plants and smart grids outperform rule-based baselines in renewable penetration and loss-of-load frequency by treating aggregations of PV, storage, and controllable loads as agents optimising long-term reward functions that combine economic, reliability, and environmental metrics [112]. Compared to static scheduling, AI-driven hybrid control in hydrogen-integrated microgrids shows better frequency regulation and lower hydrogen production costs by coordinating V2G, BESS, and electrolyser dispatch using probabilistic forecasting and RL [18]. Digital twin architectures combined with deep learning and MPC can adapt HVAC, storage, and envelope controls in buildings and urban multi-energy hubs using real-time sensor data and customised thermal comfort models. This reduces energy consumption while maintaining comfort in complex building portfolios [4]. At the local and regional level, learning-based controllers can use high-resolution predictions and state estimation to provide additional cost and emission reductions beyond deterministic MPC or heuristic DR programs. Examples of this include cloud-integrated LSTM forecasting and AI-based energy management for residential PV-battery systems, smart EV charging with PV and BESS, and digital-twin-driven health management in microgrids [105, 90, 65]. New research on multiagent DRL for UAV-assisted networks and generative AI-driven techno-economic assessment in mega-scale industrial parks suggests transferable coordination architectures that can coordinate fleets of distributed energy assets, hydrogen plants, and flexible loads across sector-coupled industrial and urban digital-twin ecosystems [24, 113, 81, 172].

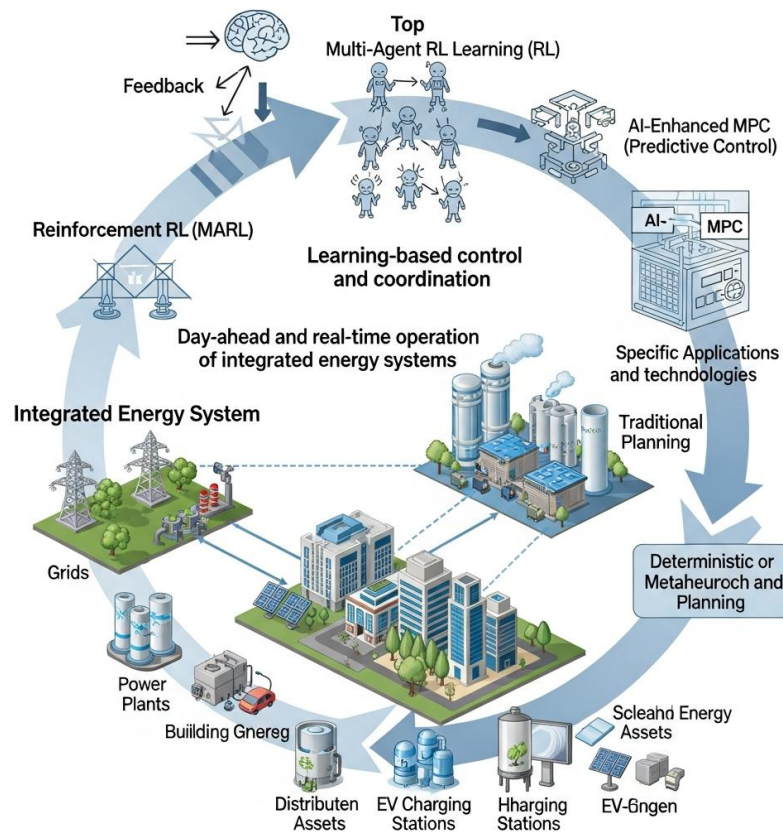


**Fig. 24.** Optimization and control solutions across typologies utilizing Learning-based control and coordination

### 6.3 Proposed Conceptual Taxonomy for AI-driven Integrated Energy Systems

As illustrated in Fig. 25, the conceptual pyramid arranges the 153-paper corpus into a taxonomy of AI-driven integrated energy system (IES) typologies at the top layer, method families in the middle, and decision layers/objectives at the base. Five typologies, A through E, are mapped as wedges in the inner ring: A: multi-energy hubs (building/district-scale couplings of electricity, heating, cooling, storage, and occasionally gas or hydrogen); B: microgrids and community systems; C: regional infrastructures spanning multi-vector electricity–gas–heat–water networks; D: sector-coupled industrial clusters (such as petrochemical, desalination, biomass–CCUS, and P2X parks); E: urban energy twins that combine digital and physical assets. Digital twin and BIM-based building portfolio optimisation and tunnels that co-optimize HVAC, thermal storage, and PV under comfort and lifecycle constraints are examples of multi-energy hubs [4, 173]. Hydrogen-integrated microgrids, redox-flow battery-stabilized weak grids, and hybrid PV–fuel-cell neighbourhood systems are examples of microgrids and communities [15]. From coordinated power-gas-heat expansion with subterranean storage to regional heat-load and PV-integration studies, regional infrastructures encompass multi-vector corridors and water-energy-waste systems [2, 106, 23]. Urban energy twins encompass smart-city digital twins for buildings, mobility, wind farms, irrigation, and public services, while sector-coupled clusters encompass IGFC/CCS plants, biomass-driven SOFC–ammonia chains, and mega-scale industrial parks [79].

In sector-coupled clusters, regional infrastructures, and multi-energy hubs, where robust formulations and MILP/MINLP support multi-vector dispatch, carbon-budgeted planning, and long-term capacity expansion, deterministic and stochastic optimisation bands are prevalent [2, 17, 166]. Microgrids, hydrogen chains, and CSP hubs are component-intensive typologies where GA, PSO, and DE wrap dryer models, CSP, and black-box PEMFCs, or advanced materials like high-capacity supercapacitors and MXene-based ionic liquids [45, 170, 46, 171]. The energy-twin and microgrid wedges have particularly thick bands of supervised/unsupervised learning and deep learning, which reflect LSTM-driven forecasting, SHAP-interpretable PV prediction, and explainable AI for building demand and emissions [105, 111, 56]. These bands span all typologies. Deep RL and multi-agent DRL optimise DR, EV charging, and task allocation under complex spatio-temporal constraints in RL/MARL bands that tighten around microgrids, virtual power plants, and UAV-enabled infrastructures [112, 113]. In multi-energy hubs, microgrids, and industrial clusters, where data-driven twins coordinate building operations, microgrid health management, and tunnel or process lifecycle optimisation, digital twins and surrogate bands are especially prevalent [4, 65, 173]. Around the materials, fluid, and structural domains, graph-based and physics-informed bands form. Explainable AI, FEM couplings, and MHD-aware neural models serve as a bridge between data-driven learning and first-principles simulations [174, 175, 50].

In multi-energy hubs, regional infrastructures, and industrial clusters, deterministic and surrogate-based bands have strong connections to planning and long-term scheduling icons. These icons are used to evaluate multi-decadal expansion, HRS network siting, and tri-objective P2X design for LCOE, LCOH, levelized desalinated water cost, and lifecycle emissions [176, 144, 62]. On the other hand, in the microgrid and mobility segments, deep-learning and RL/MARL bands thicken towards operation and real-time control icons, indicating intensive work on RL-driven EV charging coordination, LSTM-based forecasting for residential PV–BESS management, and hybrid

control for hydrogen-integrated microgrids that balance frequency regulation, cost, and state-of-charge [105, 90, 18]. Studies on RFB-regulated microgrids, autonomous maritime navigation, UAV-SCADA fire-hazard detection in solar plants, and AI-based intrusion detection for smart grids are grouped around reliability and resilience icons. Learning and stochastic control specifically target cyber-resilience, fault detection time, and loss-of-load probability [146, 141, 98, 77]. Where AI-enhanced urban mobility, smart-city decision support, and PV policy acceleration frameworks integrate accessibility, air quality, and distributional impacts alongside energy indicators, social and equity metrics are most noticeable at the edges of urban energy twins and regional planning wedges [94, 167, 168, 138, 177].

While relatively thinner RL bands in sector-coupled clusters and regional infrastructures indicate new opportunities for multi-agent RL in industrial P2X parks and cross-border transmission corridors, thick RL bands connecting microgrids, EV systems, and resilience objectives demonstrate the quick maturation of learning-based real-time control [112, 24]. In multi-energy hubs and urban twins, prominent surrogate and digital-twin bands point to a move towards closed-loop, continuously updated models that can support operational optimisation under structural change as well as long-term planning [4, 89]. The co-location of graph/physics-informed bands with deep-learning and optimisation bands in the industrial and materials segments [178, 179] shows that high-fidelity simulation and explainable AI are convergent for process intensification and structural reliability. Lastly, the explicit encoding of social and equity icons around urban and regional wedges highlights a new but expanding agenda that complements the historically predominately cost- and emissions-centric focus in energy systems optimisation by using AI-enhanced decision support to align decarbonisation pathways with fairness, affordability, and inclusion [94, 102].

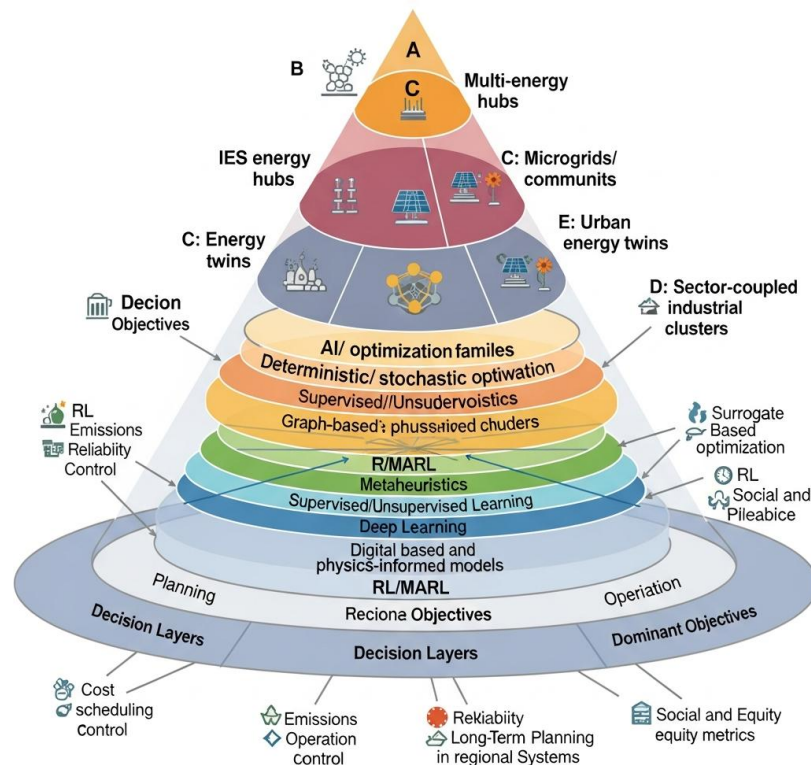


**Fig. 25.** Proposed Conceptual Taxonomy for AI-driven Integrated Energy Systems

## 6.4 Key Findings and Implications

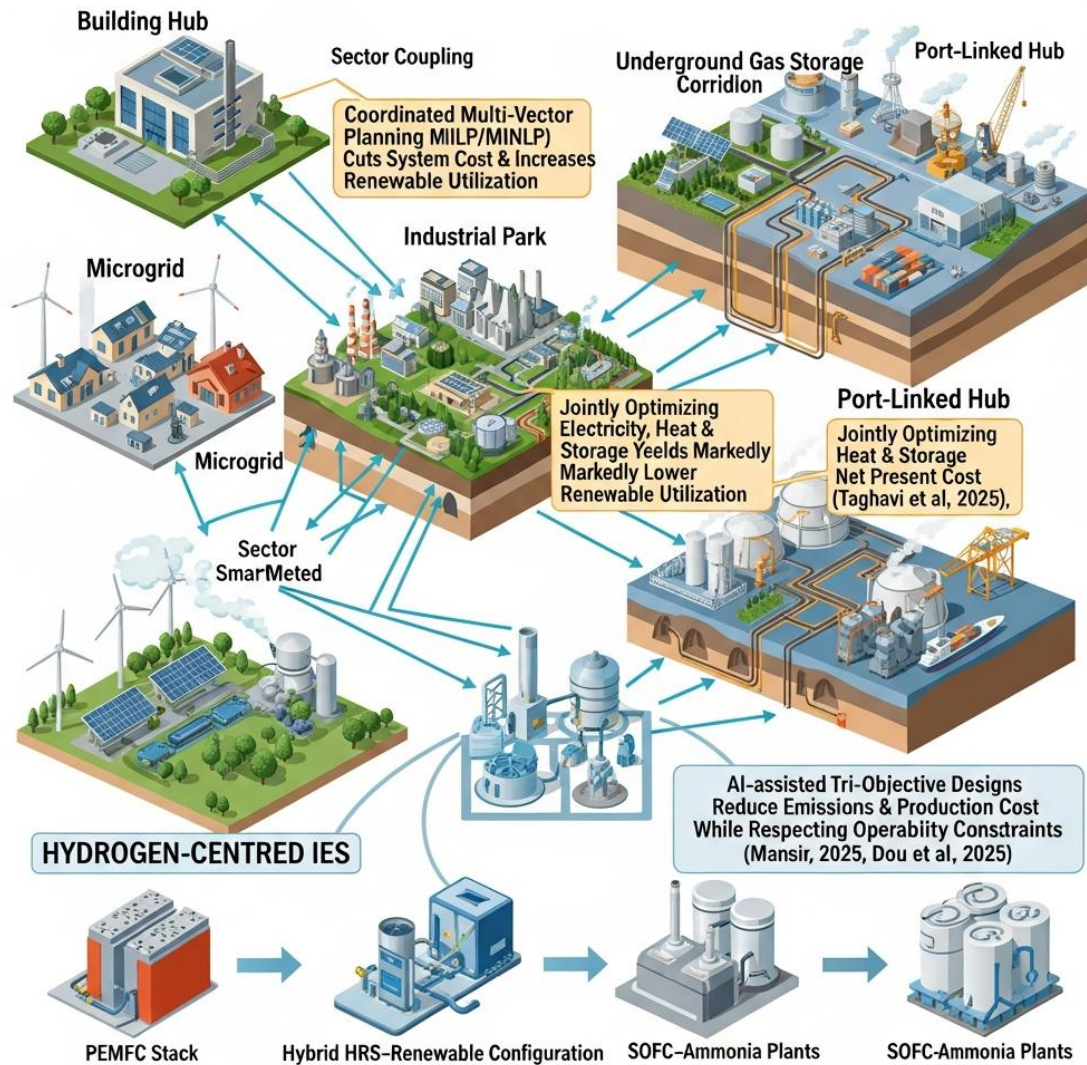


**Fig. 26.** Key Findings and Implications utilizing Techno-economic performance and efficiency of hybrid RES–H<sub>2</sub> systems

**Table 11.** Key findings and implications of AI-driven integrated energy systems across the 153-study corpus

| Cluster / theme                                                                    | Typical AI-driven IES configuration                                                       | Representative AI methods & digital tools                                                                         | Contextual & numerical performance findings                                                        | Reliability, risk & security insights                                                         | Sustainability, circularity & user-centric impacts                                                        | Key design, policy & research implications                                                                                                                                |
|------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 1. Techno-economic performance and efficiency of hybrid RES–H <sub>2</sub> systems | Multi-vector systems coupling PV, wind, batteries, hydrogen (electrolyser, FCs), CCUS and | Multi-objective metaheuristics (GA, PSO), ANN/GA hybrids, gradient-based optimisers and ML surrogates embedded in | Across hydrogen-integrated systems and solar-driven co-generation plants, AI-assisted optimisation | AI-IES designs include explicit constraints on component ratings, FC temperature windows, SoC | Coupling AI optimisers with H <sub>2</sub> , CCUS and geothermal cycles accelerates pathways towards low- | For planners and regulators, these studies show that AI-enhanced planning tools can be standardised as decision-support for tariff design, capacity-expansion studies and |

|                                                                     |                                                                                                                                                                                               |                                                                                                                                                                                                                                                                          |                                                                                                                                                                                                                                                                                                                                                              |                                                                                                                                                                                                                                                           |                                                                                                                                                                                                                                                                                          |                                                                                                                                                                                                                                                                                                                                     |
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|                                                                     | thermal units; often operated as microgrids, VPPs, or hybrid plants under market-linked tariffs.                                                                                              | techno-economic models for PV–FC hybrids, IGFC/CCS, SOFC–NH <sub>3</sub> , and geothermal H <sub>2</sub> schemes.                                                                                                                                                        | consistently identifies layouts and operating points that reduce levelised cost (LCOE/LCOH) and CAPEX/OPEX relative to rule-based baselines, typically enabling double-digit cost reductions and efficiency gains of several percentage points by co-optimising component sizing (PV, FC, tanks) and dynamic scheduling.                                     | boundaries and ramping, which improves operational robustness and reduces risk of over-stress or premature ageing in PEMFC, SOFC and storage assets.                                                                                                      | carbon industrial and power sectors, aligning hybrid systems with net-zero trajectories while improving utilisation of RES and waste-heat streams.                                                                                                                                       | investment screening, but also highlight the need for transparent multi-objective trade-offs (cost–carbon–reliability) in procurement rules and long-term contracts.                                                                                                                                                                |
| 2. Emissions reduction, carbon neutrality and circular resource use | Water-resource recovery facilities with biogas, biomass-to-bioenergy plants with CCUS, carbon-neutral buildings and net-zero water utilities that integrate PV, storage and advanced control. | AI-driven process optimisation (ANN, RL and evolutionary multi-objective algorithms) for aeration, digestion and biogas yields; XAI-based building GHG estimation; ML controllers for carbon-neutral comfort; AI-driven CCUS operation and biomass co-firing strategies. | Case studies in water facilities and biomass-integrated plants show that AI-optimised operation can raise energy recovery and biogas yields sufficiently to offset a large share of on-site electricity demand, cutting operational emissions significantly and moving systems towards facility-level carbon neutrality while maintaining process stability. | By learning from disturbance patterns and process variability, AI controllers stabilise water-treatment processes and combustion conditions, reducing flaring, N <sub>2</sub> O slips and other abnormal events that undermine environmental performance. | Building and district-scale studies report that AI-guided efficiency retrofits and deep renovation roadmaps for existing stock can unlock sizable GHG reductions, while circular-economy oriented control of biogas and biomass chains improves resource productivity and reduces waste. | The corpus points to strong policy leverage from embedding AI-based GHG accounting and optimisation into building codes, water-sector regulation and industrial decarbonisation roadmaps, while stressing the need for standards around lifecycle modelling, data transparency and verification of AI-driven carbon-neutral claims. |
| 3. Flexibility, scheduling and multi-vector energy management       | Grid-tied PV–FC–BESS hybrids, hydrogen microgrids with V2G,                                                                                                                                   | DRL and multi-agent RL schedulers for VPPs and smart grids; ANN-based EMS for PV–                                                                                                                                                                                        | Simulation and field-inspired studies show that AI-based scheduling can                                                                                                                                                                                                                                                                                      | Reliability is improved by embedding power-flow, SoC and transient-stability limits                                                                                                                                                                       | From a sustainability perspective, flexible AI-driven scheduling accelerates                                                                                                                                                                                                             | The evidence supports regulatory experimentation with AI-capable tariffs, V2G market products and interoperability standards that allow                                                                                                                                                                                             |

|                                                                       |                                                                                                                                                                                                                  |                                                                                                                                                                                                                                                 |                                                                                                                                                                                                                                                                                                                                                         |                                                                                                                                                                                                                                                                                                 |                                                                                                                                                                                                                                                                                    |                                                                                                                                                                                                                                                                                    |
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| t (microgrids, VPPs, EVs)                                             | smart EV charging hubs in dense residential districts, and DR-enabled virtual power plants coordinating flexible loads and distributed generators.                                                               | FC hybrids; probabilistic AI controllers for hydrogen microgrids; IoT-integrated EMS platforms for EV charging and building-grid coordination.                                                                                                  | significantly increase RES utilisation and reduce curtailment while flattening load profiles; DRL-coordinated VPPs and EV fleets typically achieve higher self-consumption and lower peak imports than heuristic or rule-based benchmarks, with economic gains driven by time-of-use arbitrage and reduced grid penalties.                              | directly into the reward functions and constraint sets, reducing violations during rapid RES ramps or EV charging spikes and enabling secure participation in ancillary-service markets.                                                                                                        | electrification of transport and heating while containing grid-reinforcement needs, thereby lowering lifecycle emissions and easing integration of higher PV and wind shares.                                                                                                      | DRL agents and EMS platforms to participate transparently in flexibility markets, while raising questions about explainability, algorithmic stability, and certification of RL-based controllers for safety-critical grid services.                                                |
| 4. Reliability, security and power-quality oriented AI-IES            | PV plants monitored by UAVs and SCADA, smart grids with AI-based intrusion detection, grid-connected PV with advanced power-quality analysis, and microgrids subject to cyber-physical threats and fire hazards. | Computer-vision and rough-set methods for UAV-based PV fault detection; DL-based harmonic and disturbance classification; AI-supported intrusion detection for smart grids; hybrid statistical-ML risk models for PV fire and hazard detection. | These studies demonstrate that AI can detect faults, cyber intrusions and abnormal operating conditions earlier than conventional threshold-based methods, enabling faster mitigation and reducing outage durations or damage; DL-based power-quality assessment supports finer tuning of filters, inverters and protection schemes in PV-rich feeders. | AI-enhanced monitoring improves situational awareness in PV plants and smart-grid environments, but also reveals new vulnerabilities linked to data poisoning, model spoofing and dependence on communication infrastructure, especially when AI is deeply embedded in protection or EMS loops. | Enhancing fire-hazard detection and early-warning capabilities contributes indirectly to environmental protection by reducing catastrophic asset loss and associated emissions, while secure intrusion-detection frameworks underpin public trust in digitalised low-carbon grids. | The corpus motivates coordinated standards for cyber-resilient AI-IES, including auditability of intrusion-detection models, redundancy in sensing/communication, and co-design of AI hardware, SCADA and protection to avoid single points of failure in critical infrastructure. |
| 5. Comfort, service quality and user-centric performance in buildings | Smart buildings with digital twins and advanced HVAC, carbon-                                                                                                                                                    | DT-based deep learning for personalised comfort and residential energy                                                                                                                                                                          | Building-scale studies report that AI-driven control strategies can maintain or improve                                                                                                                                                                                                                                                                 | Digital twins combined with predictive models support proactive maintenance,                                                                                                                                                                                                                    | Deep energy-renovation roadmaps for school and residential building stocks link                                                                                                                                                                                                    | Evidence points to the value of embedding AI-ready sensing, interoperability and renovation data into building regulations and performance                                                                                                                                         |

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| and cities                                                                         | neutral tropical buildings, building stock renovation planning, and assistive edge-AI systems in urban mobility and accessibility contexts.                                                                                                       | modelling; fuzzy-ML decision support for nature-based retrofits; edge inference for assistive mobility; ontology-driven AI agents for building O&M.                                                                                  | comfort while cutting HVAC energy use, often achieving noticeable reductions in cooling/heating loads in comparison with static set-point control, particularly in tropical climates and highly occupied buildings.                                                                                                                   | reducing unplanned outages of HVAC and building services, while assistive edge-AI applications demonstrate that energy-aware AI can concurrently support accessibility and safety without overwhelming local devices.                                            | AI-enabled diagnostics with long-term GHG reduction, while comfort-optimised control contributes to health, productivity and equity in high-heat or poorly insulated contexts.                                                                                                           | certificates, and of co-designing comfort-oriented AI-IES with occupant acceptance, privacy protection and equitable access in mind.                                                                                                                                                                                                                      |
| 6. Resilience and risk under geopolitical, climatic and infrastructure shocks      | National energy portfolios under gas-supply disruption, SAGIN- and 6G-enabled maritime and aerial networks underpinning logistics and energy flows, smart irrigation powered by IoT and solar PV, and microgrids with DT-based health management. | Multi-layer AI for routing and connectivity in SAGIN/6G, robust forecasting with adversarial training, DT-driven health diagnostics in microgrids, and AI-based strategic assessment of energy-security options under supply shocks. | The literature shows that AI-enabled foresight (e.g., robust heat-load or demand forecasting) and adaptive control can reduce the severity of service disruptions and improve recovery times, while strategic modelling supports diversification of supply (e.g., accelerated RES and hydrogen deployment in response to gas crises). | DT-based microgrid health management and SAGIN/6G-backed communications architectures enhance visibility and controllability during disturbances, but also introduce complex dependencies on ICT infrastructure whose failure modes must be explicitly modelled. | Climate-resilient irrigation, water-energy nexus systems and coastal energy infrastructures benefit from AI-guided adaptation strategies, helping stabilise food-water-energy services under extremes and supporting just transitions away from vulnerable fossil-centric supply chains. | Findings argue for embedding AI-based resilience planning into national energy-security strategies, with explicit attention to cascading failures, data governance and cross-border fairness, and for developing stress-tested resilience metrics tailored to AI-rich IES.                                                                                |
| 7. Cross-cutting AI/ICT enablers and digital-twin infrastructure for future AI-IES | Hierarchical edge–cloud architectures, photonic and FPGA accelerators, federated LoRaWAN and 6G/NTN networks, and domain-specific digital twins for buildings and microgrids.                                                                     | Photonic accelerators, STT-MRAM in-memory computing, FPGA-based NN engines, federated learning for far-edge IoT, integrated sensing–communication–computation, and ontology-enabled DT platforms for O&M and health                  | Benchmarks demonstrate that specialised AI hardware and edge/federated schemes can deliver low-latency inference with reduced computing energy, enabling real-time control, forecasting and fault detection in AI-IES                                                                                                                 | Distributed AI and DTs reduce single-point-of-failure risks relative to highly centralised EMS, but raise new challenges around synchronisation, model versioning and secure aggregation in federated settings;                                                  | As AI accelerators, edge networks and digital twins become more energy-efficient themselves, they form an enabling substrate for pervasive AI-IES, while also demanding careful accounting of their own                                                                                  | The corpus underlines the importance of treating AI/ICT infrastructure as part of energy-policy debates: standardisation around open, interoperable DT platforms, governance of federated and edge AI, and alignment of ICT roadmaps with net-zero strategies are all necessary conditions for scalable, trustworthy AI-driven integrated energy systems. |

|  |  |             |                                                                                                                                                                              |                                                                                                   |                                                               |  |
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|  |  | management. | without prohibitive cloud dependence; cloud-integrated LSTM forecasting frameworks exemplify how such infrastructure supports high-resolution residential energy management. | timing-guarantee work for embedded AI shows how real-time constraints can be rigorously enforced. | embodied and operational footprints to avoid rebound effects. |  |
|--|--|-------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------|---------------------------------------------------------------|--|

The crucial role that learning-based forecasting, control, and digital twins play in releasing operational value in AI-driven IES is a second cross-cutting finding. When compared to deterministic scheduling under perfect-forecast assumptions, residential and community energy management frameworks that combine LSTM solar and demand forecasts with cloud-integrated EMS consistently demonstrate lower energy bills and curtailed peaks. This indicates that predictive capability and decision logic need to be co-designed rather than treated separately [105], as illustrated in Fig. 27. Digital-twin platforms for microgrids and buildings simulate thermal dynamics, equipment deterioration, and occupant comfort using statistical machine learning and deep learning. This allows for ongoing recalibration of MPC setpoints and maintenance schedules while maintaining manageable data requirements [115, 65]. Deep reinforcement learning and hybrid stochastic-RL controllers outperform rule-based baselines in microgrids, virtual power plants, and EV charging districts in terms of renewable hosting and frequency stability, particularly when PV and EV demand are highly volatile [112, 90, 18]. Further evidence that combining semantic models with AI agents enhances fault detection, maintenance prioritisation, and comfort-energy trade-offs in complex portfolios comes from intelligent building operations and ontology-enabled twins [166, 138]. These developments suggest that future IES architectures' control hierarchies will more closely resemble closed-loop digital ecosystems, where forecasters, RL agents, and surrogates with knowledge of physics collaborate to influence both day-ahead and real-time decisions.

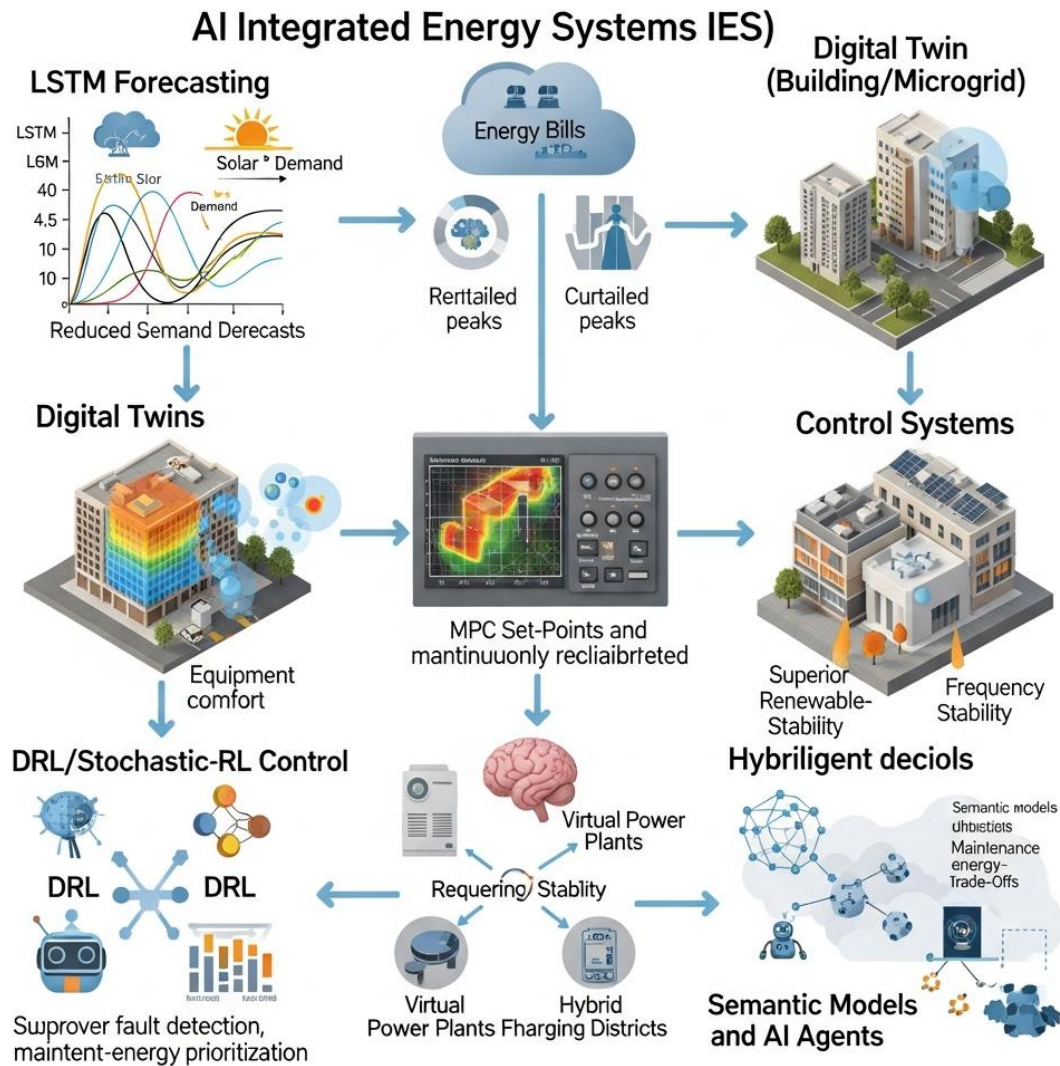


**Fig. 27.** Key Findings and Implications utilizing central role of learning-based forecasting, control and digital twins

Wastewater treatment plants are positioned as dispatchable low-carbon resources in regional systems [17, 82], and water-energy-waste facilities using AI-optimized biogas production and pump scheduling show how circular flows can drive plants towards carbon-neutral operation while respecting hydraulic constraints and service reliability (Fig. 28). Geothermal–desalination–hydrogen and biomass-to-bioenergy schemes demonstrate how ML-assisted process design can recover otherwise wasted heat and energy, increasing the feasible decarbonisation space in industrial clusters [139, 43]. According to Reis et al. [94], Bibbò et al. [95], Banluesapy et al. [122], Huang et al. [89], and others, intelligent irrigation systems, generative spatial AI for urban digital twins, and AI-enabled mobility platforms show how coordinated optimisation of logistics, transportation, and green infrastructure can lower emissions while increasing service accessibility and water productivity in urban areas. AI-driven IES models inform tariffs, incentives, and standards at scale, and policy-oriented frameworks that use AI to speed

up PV adoption, assess smart-building regulations, or create hydrogen investment programs indicate a move away from purely technical optimisation and towards evidence-guided policy analytics [168, 92, 138]. It is implied that AI-driven IES research is moving from the optimisation of individual assets to systemic interventions that affect governance, ecosystems, and infrastructure all at once.

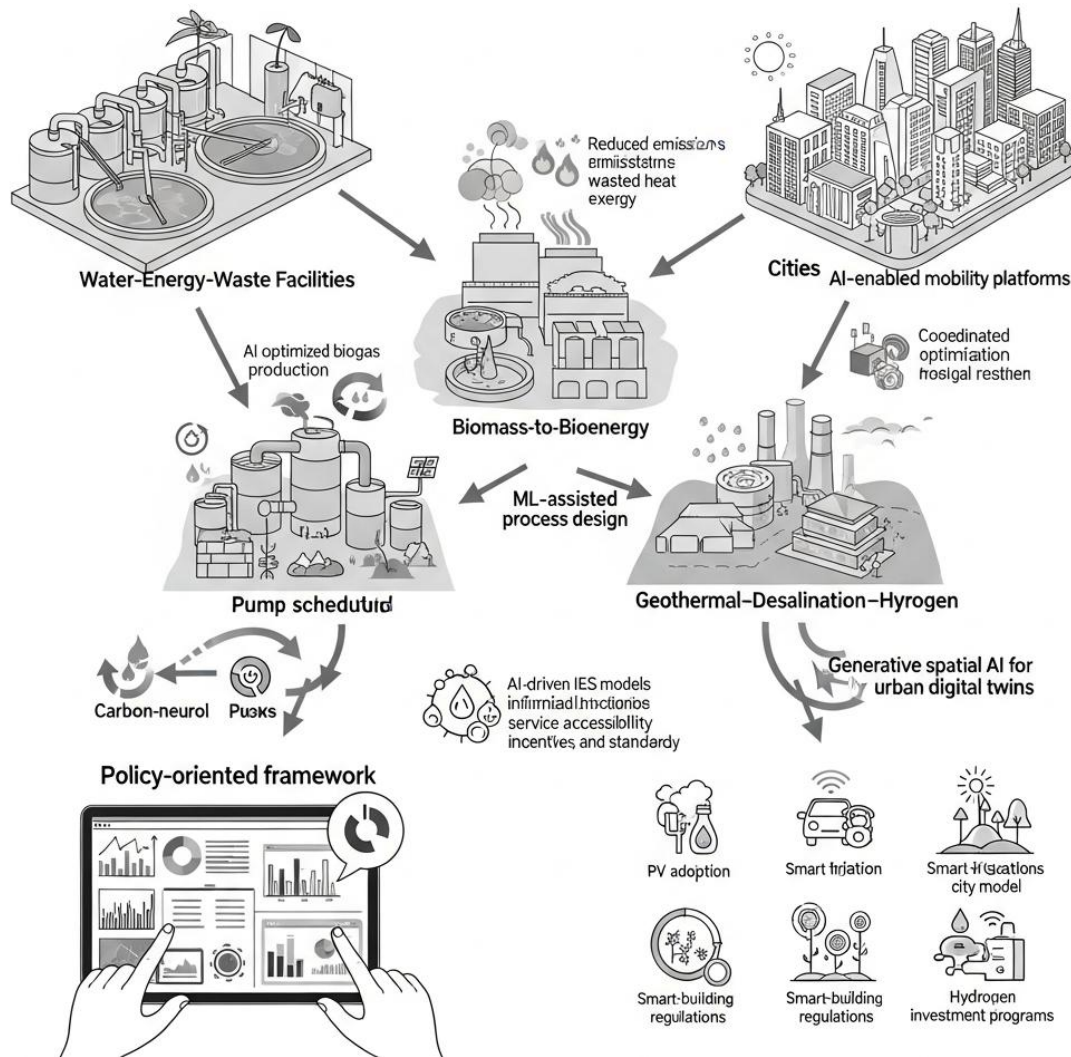


**Fig. 28.** Key Findings and Implications utilizing integrative levers for circularity, sector coupling and multi-benefit urban transitions

Lastly, research reveals significant governance, infrastructure, and risk implications that reduce the excitement surrounding AI-driven IES. Numerous studies highlight how integrating AI into sensing, communication, and control layers increases the cyberattack surface. Examples of this include reviews of blockchain-secured automation, critical infrastructure vulnerability assessments, and smart-grid intrusion detection work [98, 70, 69], as depicted in Fig. 29. The computational substrate of IES is rapidly moving towards ultra-dense, heterogeneous hardware, with timing guarantees and energy efficiency becoming design constraints in and of themselves. edge and 6G-enabled architectures for far-edge IoT, photonic accelerators, and low-latency AI for

metaverse-scale applications [68, 126, 66, 180] are examples of this. AI-centred optimisation can significantly impact geopolitical resilience, but it also runs the risk of lock-in if models incorporate antiquated fuel prices or policy assumptions, as demonstrated by case studies on Germany's AI-driven energy security strategy and massive petrochemical industrial parks [102, 24]. This can be done through explainable models, physics-consistent surrogates, cyber-secure communication stacks, and inclusive policy co-design.

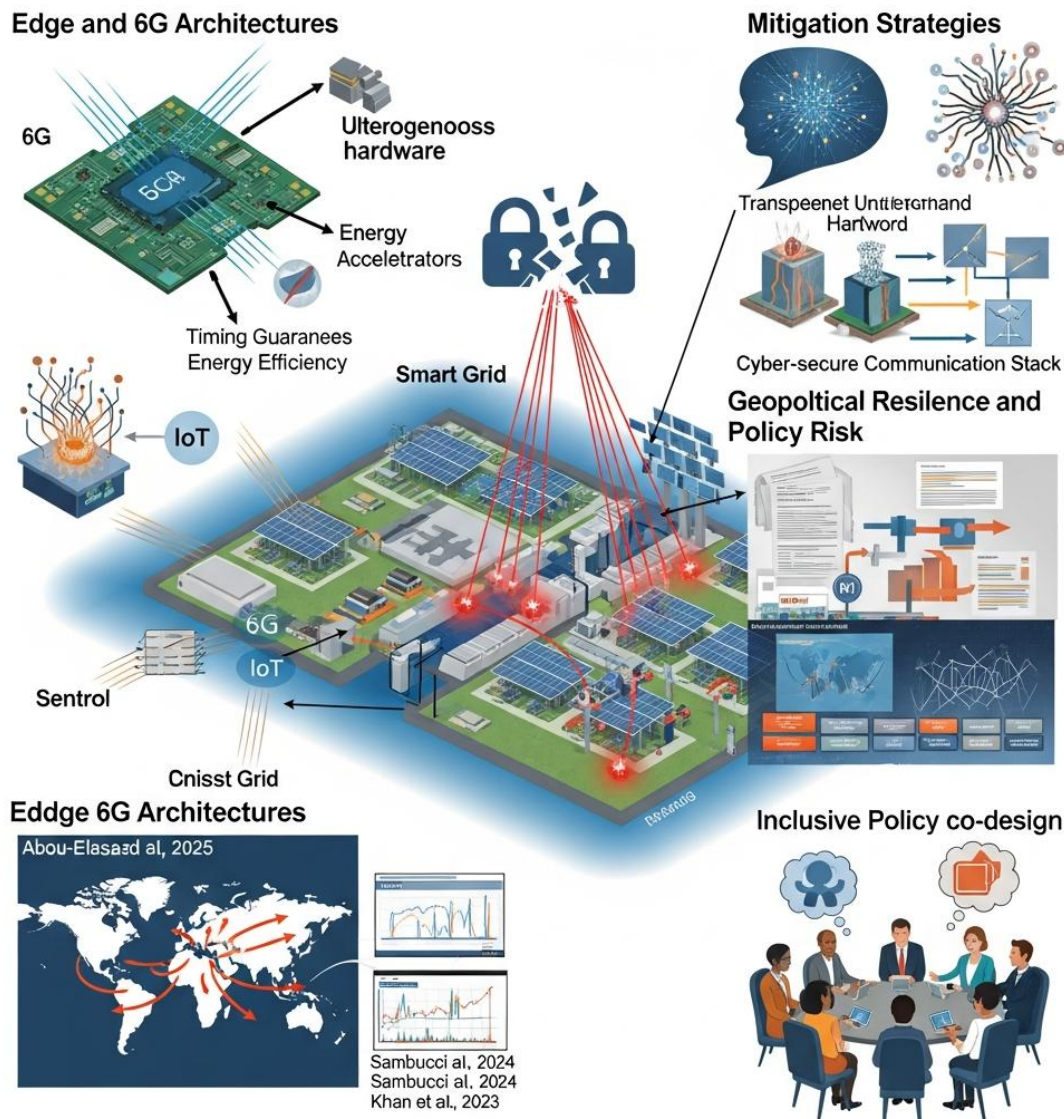


**Fig. 29.** Key Findings and Implications utilizing risk, infrastructure and governance implications

## 8. Emerging Trends, Research Gaps, and Global Roadmaps (2030 -2050)

### 8.1 Emerging Trends and Research Gaps in Ai-Driven Integrated Energy Systems

As shown in Table 12, digital-twin and surrogate-based AI architectures are quickly evolving into the "control rooms" of AI-driven integrated energy systems (AI-IES), allowing for high-fidelity virtual representations of buildings, districts, and microgrids that are constantly in sync with sensor streams and market data. As evidenced by twin-driven residential energy modelling and personalised thermal comfort control for smart buildings, residential and commercial building twins already combine intricate physics-based models with machine-learning surrogates to co-optimize thermal comfort, HVAC scheduling, and electricity use [115, 86]. Digital-twin frameworks for building operations and maintenance bridge the gap between BIM, SCADA, and control layers in near real time by structuring asset hierarchies, fault signatures, and control actions using ontology-enabled AI agents [166, 173]. By integrating prognostics and diagnostics into cyber-physical replicas, digital-twin-driven health management of microgrids and grid assets at the network scale allows for proactive maintenance and resilience planning [65, 51]. Surrogate models are increasingly driving these twins: GAN-based surrogates simulate year-round weather and PV production for reliable grid integration studies [23, 110], while process-simulation surrogates for green dimethyl ether and biomass-SOFC–ammonia plants speed up tri-objective techno-economic–environmental optimisation [80, 62]. A second developing strand is reinforcement learning (RL) and multi-agent RL (MARL), especially in situations where AI-IES must negotiate multi-objective trade-offs and multi-actor interactions in the face of uncertainty. In virtual power plants and smart grids, deep RL has been specifically used to co-optimize renewable penetration, operating costs, and grid stability by framing demand response and dispatch as sequential decision problems subject to network physics constraints [112]. This reasoning is extended in multi-agent DRL to prosumer households, fleets of EV chargers, and flexible industrial loads. In these scenarios, agents compromise system-level restrictions on feeder loading, congestion, and emissions while negotiating local goals (such as charging convenience and device degradation) [90, 113]. In order to manage electrolyzers, fuel cells, and vehicle-to-grid interfaces in the face of stochastic renewables, price signals, and mobility patterns, hydrogen-integrated microgrids and refuelling infrastructures also use learning-based hybrid controllers [18, 3, 48]. Intelligent EV-charging hubs and AI-optimized regenerative braking in electric buses exhibit RL-style adaptation to traffic conditions and tariff dynamics in congested urban corridors, preserving grid reliability and passenger service [91, 181]. These studies collectively demonstrate a move away from static rule-based energy management and towards self-learning controllers that can encode risk-aware strategies and increase the use of renewable energy sources without jeopardising supply security. A third major trend that addresses the shortcomings of purely data-driven approaches in safety-critical, data-sparse energy environments is the use of hybrid and physics-informed AI models. As demonstrated by AI-driven PEMFC optimisation, PEMFC flow-field design, adsorption chillers, and direct solar dryer configurations, numerical CFD and electrochemical models are increasingly combined with neural surrogates or metaheuristic optimisers in fuel cells and thermal systems to explore large design spaces under stringent physical constraints (Ayadi et al. [45]; Jiang et al. [126]; [49]; Loksupapaiboon et al. [118]). Explainable AI is directly integrated into constitutive modelling and finite-element analysis in structural and materials-oriented

energy applications, such as advanced aerogels, neuromorphic devices, and coal gangue concrete, which must concurrently meet mechanical, thermal, and safety requirements [116, 149, 112]. Machine-learning-accelerated design of fractured geothermal systems and geothermal-integrated hydrogen production in subsurface and thermal networks combines ML surrogates with first-principles simulators to produce multi-objective designs that adhere to reservoir behaviour and thermodynamic bounds [179, 43]. The hybrid cyber-physical models for micro gas turbines, redox-flow batteries, and combined heating/cooling loops [160, 77] show how incorporating domain equations into learning architectures improves sample efficiency, extrapolation, and trustworthiness—all essential requirements for AI-IES to function closer to technical limits [182-191].

A fourth trend is the use of distributed and privacy-preserving AI architectures, which allow for the widespread deployment of AI-IES without the need to centralise sensitive data or strain communication infrastructure. It is shown that models can be trained or updated locally at far-edge devices with only low-dimensional parameters or gradients shared by edge AI and federated learning frameworks designed for 5G/6G, LoRaWAN, and space-air-ground integrated networks [66, 68, 192]. These methods are directly applicable to EV fleets, building clusters, and microgrids where privacy issues are brought up by load profiles, occupancy patterns, and mobility traces. AI-based wireless sensor IoT networks and resource-efficient edge inference systems demonstrate how limited devices can host anomaly detection, forecasting, or control policies for PV systems, wind farms, and consumer electronics without relying on the cloud [158, 193, 96]. Meanwhile, AI-aided 6G maritime or SAGIN architectures and AI-enabled integrated sensing-communication-computation platforms demonstrate how energy, communications, and computation can be co-designed to support distributed optimisation across large areas [19]. Cybersecurity-focused research on AI-plus-blockchain frameworks for safe power distribution and AI-based intrusion detection for smart grids highlights that privacy, integrity, and robustness are emerging as top design goals in AI-IES rather than afterthoughts [98, 69].

Circular economy-aligned energy systems that reduce emissions and valorise wastes include net-zero water-sector pathways, biomass-to-bioenergy with carbon capture, and AI-driven optimisation of biogas-centred water resource recovery facilities [17, 82, 139]. Integrated energy-water systems for desalination and wastewater-to-bioenergy use AI to lower emissions and energy intensity in the face of rising water stress, particularly in arid regions [84, 83]. AI-optimized smart buildings, nature-based decision support for building projects, and AI-informed PV policy design in Lisbon demonstrate how data-driven tools can socially sensitively address fuel poverty, retrofit priorities, and urban heat-island risks at the urban and regional level [168, 138, 88]. Rural smart-irrigation microgrids that use solar power and artificial intelligence (AI), hybrid renewable microgrids, and hydrogen systems—which match resilience and dependability with livelihoods—extend these advantages to agricultural and remote communities [122, 64, 133]. However, research on national energy security plans, critical infrastructure vulnerabilities, and AI-enabled industrial parks highlights that AI-IES needs to be specifically designed with consideration for distributional effects, geopolitical shocks, and climate extremes [24, 70, 102]. Together, these threads point to a developing field of study in which AI-powered integrated energy systems progress from discrete technical improvements to socio-technical infrastructures that are physics-based, privacy-preserving, cyber-secure, and specifically focused on energy justice and climate resilience [194-196].

**Table 12.** Emerging trends and research gaps in AI-Driven integrated energy systems

| Emerging trend in AI-Driven IES                       | Conceptual focus & novelty                                                                                                                                                                                                                                                                                                                                                                          | Core AI / analytics methods                                                                                                                                                                                                                                                                          | Targeted systems & energy vectors                                                                                                                                                                                                                                         | Illustrative applications & case studies                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | Main performance / sustainability insights                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        | Open research gaps & future directions                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
|-------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Digital-twin and surrogate-based AI architectures     | Digital twins (DTs) and AI surrogates turn integrated energy systems into continuously calibrated virtual replicas that fuse physics-based models with real-time sensor data. The novelty lies in multi-scale coupling: component-level electrochemistry, building thermodynamics and network flows are abstracted into fast, differentiable AI models that remain anchored in engineering reality. | Deep neural surrogates trained on detailed simulators, statistical ML for parameter calibration, autoencoders for state compression, and generative models for scenario synthesis. DT frameworks often embed ontologies and knowledge graphs to orchestrate models and data across lifecycle phases. | Building and district multi-energy hubs (electricity–heat–cooling), microgrids with storage and EVs, microgrid health monitoring, and city-scale energy–mobility platforms. Vectors typically include electricity, heating/cooling and sometimes hydrogen or water flows. | Residential digital twins combining statistical ML with building physics to co-optimize comfort and electricity use [4]; deep-learning-based DT for personalised thermal comfort and efficient building operation [4]; ontology-enabled AI agents for building O&M twins that can be composed into larger urban twins [166]; DT-driven health management in microgrids to anticipate failures and reconfigure topologies [65]; generative spatial AI as the core of urban digital twins for sustainable smart cities [89]; GAN-based surrogates for PV integration studies that generate realistic year-round weather series to probe hosting capacity [23, 110]; digital-twin-inspired virtual frameworks for LSTM-driven solar forecasting and residential energy management [105]. | Across these studies, DT–AI hybrids achieve orders-of-magnitude faster simulations than high-fidelity solvers while keeping sufficient accuracy for optimisation and control, enabling real-time reconfiguration of building HVAC, microgrid dispatch and PV hosting decisions [4, 65]. Generative models allow planners to explore extreme yet plausible climate and demand futures, stress-testing city-scale energy plans beyond historical records [89, 110]. DT-based health management reduces unplanned outages and extends asset lifetime by coupling diagnostics with reconfigurable control actions in microgrids [65]. | Key gaps include interoperable DT standards across vendors and sectors, robust validation of AI surrogates under out-of-distribution climate and operational regimes, and embedding cyber-security and privacy-by-design into DT stacks that span buildings, grids and industrial clusters [17]. There is also a need for open reference DTs and benchmark datasets for typical integrated energy archetypes—residential neighbourhoods, hydrogen hubs, ports—to move from bespoke one-off implementations to reproducible, comparative science [216]. |
| Reinforcement learning (RL) and multi-agent RL (MARL) | RL reframes energy management as sequential decision-making under uncertainty, where controllers learn optimal actions (dispatch, charging, set-points) by interacting with simulated or real environments. MARL extends this to collections of interacting agents—buildings, EV fleets, microgrids, UAVs—negotiating shared resources and grid constraints.                                        | Deep RL (e.g., actor–critic, DQN) for continuous control; multi-agent DRL with shared or local critics; policy-gradient algorithms for multi-objective optimisation; generative and model-based RL where learned environment models reduce sample complexity.                                        | Virtual power plants that aggregate distributed resources, multi-energy microgrids with hydrogen and V2G, EV–PV–BESS charging districts, and cyber-physical systems where UAVs, sensors and edge devices cooperate over 5G/6G networks to support energy services.        | Deep RL for multi-objective optimisation in virtual power plants and smart grids, maximising renewable integration and grid efficiency while respecting security constraints [112]; AI-driven hybrid control for hydrogen-integrated microgrids with probabilistic energy management and V2G interactions, providing a natural substrate for RL-based policy learning [18]; AI-driven optimisation of smart EV charging systems coupled with PV and BESS in dense residential areas, where charging schedules can be cast as RL tasks with network constraints [90]; generative AI-driven multi-agent DRL for task allocation in UAV-assisted networks that support sensing and communication for energy-critical infrastructures [113]; coordinated multi-vector management with     | These works show that RL controllers can internalise complex nonlinearities and constraints that are difficult to encode in rule-based schemes, such as the interaction between hydrogen storage, V2G and stochastic renewables in microgrids [18]. For VPPs, DRL identifies dispatch strategies that balance curtailment minimisation, congestion relief and revenue, outperforming static heuristics under volatile market conditions [112]. MARL in UAV-assisted and SAGIN contexts offers a blueprint for distributed coordination of sensing, communications and                                                             | Open challenges include safe RL under strict grid codes and protection constraints, sample-efficient training that avoids excessive experimentation on real assets, and transparent reward designs that encode both engineering limits and societal objectives. MARL in large-scale systems faces issues of non-stationarity and scalability, requiring new abstractions to aggregate agents without losing critical local dynamics [217]. There is a growing need to couple RL with domain-knowledge                                                  |

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|                                                     |                                                                                                                                                                                                                                                                                                                                                               |                                                                                                                                                                                                                                                                                                                           |                                                                                                                                                                                                                                                               | underground storage and AI-based maritime scheduling, pointing toward RL-ready formulations of coupled port–grid–shipping systems [2].                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | energy services, crucial for resilient monitoring of remote renewables and grids [113].                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | constraints and to verify learned policies against worst-case disturbances and cyber-attacks [213, 70].                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |
| Physics-informed and hybrid AI models               | Physics-informed and hybrid AI fuse first-principles models (thermodynamics, electrochemistry, fluid dynamics) with data-driven learning, aiming to retain interpretability and extrapolation ability while capturing unmodelled complexities. This trend is central for AI-IES because integrated systems couple multiple physical domains over wide scales. | Physics-informed neural networks that incorporate governing equations as soft constraints; hybrid grey-box models that combine mechanistic cores with ML residuals; explainable AI aligned with finite-element and CFD solvers; meta-modelling where ML accelerates high-fidelity simulators for design and optimisation. | Fuel cells and electrolyzers, geothermal and adsorption-based thermal systems, advanced materials in PV and storage, SOFC-based power-to-X plants, and microgrid components whose dynamic behaviours are partly known but difficult to calibrate in practice. | Global–local explainable AI tightly coupled with finite-element validation for constitutive modelling of coal gangue concrete, illustrating how structural physics and AI co-produce reliable material models [116]; ML-accelerated multi-objective design of fractured geothermal systems, where hybrid models reduce the evaluation burden of complex subsurface physics [179]; adsorption chiller simulations enhanced by neural networks, enabling faster exploration of combined heating and cooling system configurations [49]; emission forecasting in automotive systems that integrates experimental data with neural computation, demonstrating hybrid learning from physics-guided features [143]; AI-assisted tri-objective optimisation of biomass-driven SOFC electricity–ammonia plants that builds on detailed process models [62]; solar-driven hydrogen and co-generation systems optimised through AI while respecting thermodynamic and electrochemical constraints [144, 81]. | Hybrid approaches consistently show superior data efficiency and robustness compared to purely black-box models, especially when extrapolating beyond the training range—crucial for long-term climate and policy scenarios [179, 62]. Embedding conservation laws and feasible operating regions into learning architectures reduces physically impossible predictions and aids operator trust, facilitating deployment in safety-critical hydrogen and SOFC clusters [144]. For materials and thermal systems, physics-guided networks accelerate design loops while preserving linkages to underlying mechanistic parameters, enabling multi-scale optimisation from device to system level (Dong et al. [174]; [49]). | Remaining gaps include standard frameworks for encoding partial physics knowledge into ML architectures across different carriers (electricity, heat, hydrogen), rigorous uncertainty quantification that propagates both data and model errors, and methods to manage “physics wrong but useful” models when legacy equations clash with new operating envelopes. There is also a need for shared benchmark problems that compare pure data-driven, pure physics and hybrid approaches under identical conditions, especially for complex multi-vector systems such as power-to-X hubs and integrated desalination–energy plants [84, 43]. |
| Privacy-preserving and distributed AI architectures | As IES become dense cyber–physical networks, data sovereignty, latency and reliability push AI from centralised clouds toward federated and edge-centric deployments. Emerging architectures seek to learn from distributed data—across buildings, feeders, districts and organisations—without                                                               | Federated learning across far-edge IoT nodes; resource-efficient edge inference; compressed and quantised neural networks for embedded devices; AI-enabled 6G and LoRaWAN stacks; blockchain-                                                                                                                             | Smart-city scale sensing layers, distributed PV and wind farms, microgrids with extensive IoT instrumentation, and critical grid infrastructure where on-site inference is essential for safety and privacy.                                                  | Resource-efficient federated LoRaWAN architectures for far-edge IoT applications, providing a blueprint for distributed learning over constrained radios in smart-city and energy contexts [68]; surveys and frameworks for AI-enabled integrated sensing, communication and computation that anchor distributed AI in next-generation networks [19]; sustainable 6G architectures geared to align communication networks with energy and carbon targets [66]; AI-aided integrated terrestrial–non-terrestrial 6G for maritime                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | Distributed AI architectures lower latency for protection and control, improve robustness to backhaul outages, and reduce privacy risk by avoiding raw data centralisation—vital for household-level load profiles, mobility traces and industrial process data [193, 68]. Federated and edge AI support massive scaling of sensors in smart cities and renewables without proportionally increasing communication energy                                                                                                                                                                                                                                                                                                 | Major research needs include robust aggregation schemes for non-iid and sparse energy data, incentive-compatible data sharing across utilities and prosumers, and formal privacy guarantees aligned with evolving regulations. Interactions between AI workloads and network energy consumption require co-optimised designs                                                                                                                                                                                                                                                                                                                |

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|                                               | centralising sensitive information, while exploiting 5G/6G and SAGIN connectivity.                                                                                                                                                                                                                                                                                                                     | supported data integrity; intrusion detection and anomaly detection models tailored to constrained hardware.                                                                                                                                                                                                                                      |                                                                                                                                                                                                                                   | networking, relevant to offshore renewables and shipping corridors [136]; deep-learning-based B5G open RAN designs that enable flexible, programmable edge intelligence (Bouziane et al., 2022); edge-focused studies of DNN deployment on AI accelerators [218] and edge inference assistance systems [158]; AI-based wireless IoT sensor networks for energy-efficient electronics [193]; AI-based smart-grid intrusion detection [98, 213] and blockchain-secured smart grids [69].                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          | use, aligning digitalisation with sustainability [66]. Integrated intrusion detection and blockchain-based integrity mechanisms help harden AI-IES against cyber-attacks, particularly in highly automated, AI-dependent grids [98, 69].                                                                                                                                                                                                                                                                                                                                                                                                                         | where energy, communication and computation are treated jointly [19]. Finally, there is a critical need for testbeds that combine federated learning, 6G links and real energy devices to evaluate resilience under faults and adversarial attacks [70].                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
| Climate-resilient and justice-oriented AI-IES | A growing strand of work reframes AI-IES not only as tools for efficiency and cost minimisation, but as instruments for climate resilience, just transitions and social inclusion. This involves embedding resilience metrics, environmental externalities and equity considerations into optimisation objectives, and using AI to design policies that prioritise vulnerable regions and communities. | Multi-objective and multi-criteria decision models that internalise resilience, emissions and equity; generative scenario analysis for climate and policy shocks; spatial AI for vulnerability mapping; policy-analytics platforms that connect micro-level optimisation with macro-level distributional impacts; governance-aware AI frameworks. | Net-zero water–energy–waste infrastructures, biomass-to-bioenergy and CCS clusters, smart and inclusive cities, hydrogen and HRES roadmaps, and critical-infrastructure protection in the face of climate and geopolitical risks. | AI-driven optimisation frameworks that enhance energy circularity and carbon neutrality in water resource recovery facilities, tying biogas production to net-zero strategies [17]; application of AI in net-zero carbon water sector case studies [82]; generative-AI-enabled assessment of mega-scale decarbonised industrial parks integrating renewables and sustainable energy vectors [24]; AI-integrated biomass-to-bioenergy management and carbon capture to achieve carbon neutrality [139]; integrated energy informatics for microalgae-based wastewater-to-bioenergy systems [83]; AI-based PV policy frameworks aimed at accelerating equitable solar deployment in Lisbon [168]; smart-city AI decision-support that targets sustainable energy management [167] and energy-aware low-emission urban mobility [94]; AI-augmented smart irrigation using IoT and solar power to manage water–energy trade-offs in agriculture [122]; analyses of AI-driven energy systems within national energy security strategies such as Germany’s gas exit [102]; reviews of HRES pathways with hydrogen, biomass and solar for low-carbon transitions [64]. | These studies collectively show that AI-IES can unlock climate co-benefits beyond pure efficiency, such as circular resource use, deep decarbonisation of hard-to-abate sectors, and resilient operation of water–energy systems under climate extremes [17, 209]. Urban cases demonstrate that AI-guided planning of mobility, buildings and green infrastructure can reduce emissions while improving service access and liveability [94, 167]. Policy-oriented work highlights how AI analytics can inform strategic decisions like gas-phase-outs, hydrogen investments and biomass siting, potentially reducing stranded-asset and lock-in risks [102, 64]. | Research gaps include systematic integration of distributional equity metrics—who benefits, who bears risks—into AI optimisation, building on lessons from AI ethics in other domains [111]. There is a need for climate-stress testing of AI-IES under compound extremes (heatwaves, droughts, supply shocks) and for coupling physical resilience (redundancy, flexibility) with cyber-resilience against coordinated attacks [70]. Finally, participatory and transparent AI tools are required so that communities, regulators and utilities can co-design transition pathways, ensuring that AI-accelerated decarbonisation aligns with justice and inclusion objectives rather than exacerbating existing inequalities [168, 138]. |

## 8.2 Global Roadmap for Ai-Driven Integrated Energy Systems (2030-2050)

As shown in Table 13, Phase I of the roadmap (2026–2030) builds on the current wave of reliable pilots that employ AI to encapsulate local networks and individual assets

with strong digital representations prior to attempting system-wide autonomy. The methodological basis for large-scale AI-driven integrated energy systems (AI-IES) is already being laid by digital-twin platforms for buildings and microgrids, which show how high-fidelity models combined with statistical and deep learning can produce verifiable improvements in comfort, energy efficiency, and fault detection. In order to calibrate residential energy models and customised thermal comfort in smart buildings, Almadhor et al. use digital twins and machine learning. This allows them to create a template for KPI-driven pilots that specifically monitor comfort, energy savings, and model uncertainty [115]. By employing digital twin-driven health management to monitor dispersed assets and predict failures, Ebrahimi et al. expand the twin concept to microgrids, meeting the cyber-physical security standards for future autonomous grids [65]. In parallel, the predictive backbone needed for adversarially robust forecasting for regional heat loads and solar resource availability using sophisticated data-driven techniques is created by adversarially robust forecasting [106, 105]. Currently being investigated in limited environments with multi-objective formulations for grid efficiency and renewable integration, deep reinforcement learning for virtual power plants and smart grids offers an early blueprint for how AI agents will balance cost, reliability, and emissions in these pilots prior to their scaling [112]. These initiatives collectively suggest a 2026–2030 period in which reliable, standards-aligned testbeds concentrate on digitalisation at the asset and microgrid levels, thorough benchmarking, and risk-aware RL deployment in operational domains that are carefully fenced [197].

According to the roadmap, these discrete pilots will knit into scaled, interoperable, and human-centric AI-IES that cut across industries and jurisdictions by Phase II (2030–2040). Evidence from cross-sectoral AI optimisation in water, buildings, and industrial systems demonstrates how integrated data and control layers can support decarbonization at the infrastructure scale. Farzin et al. provide a model for water–energy–waste coupling in regional IES architectures by showcasing AI-driven optimisation frameworks that employ biogas generation in water resource recovery facilities to improve energy circularity and advance towards carbon neutrality [17]. Ramos et al.'s case-study pathway for net-zero carbon water utilities serves as an example of the integration of AI-enabled monitoring and decision support into regulated service environments [82]. As demonstrated by Huang et al.'s large-flow model for sustainable cities, which integrates infrastructure, mobility, and land use into a single AI–DT stack, generative spatial AI and urban digital twins start to function as "operating systems" for smart cities at the urban scale [89]. As AI-driven EV charging frameworks integrated with PV and BESS in dense residential areas [90] and AI-optimized comfort control in tropical buildings [86] prioritise user comfort, charging equity, and local grid stability as co-equal goals rather than side constraints, human-centricity becomes clear. Systematic reviews of AI-enabled decision support for sustainable smart cities [167] and hybrid renewable energy systems [64] support this scaling phase. These reviews provide the design patterns, benchmarks, and taxonomy required for standards-compliant, interoperable AI-IES platforms that can connect to edge-AI, 5G/6G, and SAGIN infrastructures.

With the help of new research on security, energy justice, and climate-resilient infrastructure, the roadmap's last phase, Phase III (2040–2050), aims to create autonomous, resilient, and justice-oriented AI-IES. In light of the Russian gas exit, current analyses of AI-driven energy security strategies demonstrate how demand response, diversified low-carbon supply, and flexibility portfolios enabled by AI can all help to reduce geopolitical shocks while adhering to environmental policy restrictions

[102]. Simultaneously, research on AI and critical infrastructure vulnerabilities highlights the necessity of continuous adversarial risk assessment and secure-by-design architectures [70, 98], while secure smart-grid schemes enabled by AI and blockchain demonstrate how integrity, traceability, and privacy can be deeply ingrained in grid protection layers [69]. AI-augmented smart irrigation driven by solar PV in water-stressed regions [122] and AI-based decision frameworks to speed up equitable PV deployment in cities like Lisbon [168] foreshadow justice-oriented AI-IES trajectories, where socioeconomic heterogeneity and policy constraints are key design variables rather than ex-post considerations. According to the roadmap, by 2040–2050, mature AI-IES will function as self-healing, climate-aware, and socially aligned infrastructures: digital twins mediating multi-sector flows (food, water, energy, and mobility); reinforcement learning agents coordinating across market and jurisdictional boundaries; and governance frameworks that institutionalise participation, transparency, and reparative investment in historically underserved regions. The corpus indicates that future AI-IES will be evaluated on their ability to close equity gaps in access, affordability, and environmental quality while sustaining communities under a series of climate and geopolitical shocks, rather than just optimising energy metrics [198].

**Table 13.** Global roadmap for AI-Driven integrated energy systems (2030-2050)

| Roadmap phase & horizon                               | Strategic focus and system archetypes                                                                                                                                                                                                                                                                                                                                                                                            | Dominant AI paradigms & digital stack                                                                                                                                                                                                                                                                                                                                                                                                          | Key capabilities & performance targets                                                                                                                                                                                                                                                                                                                              | Representative application domains                                                                                                                                                                                                                                                                                                                                      | Research & implementation priorities (2030–2050)                                                                                                                                                                                                                                                                                                                                                                  | Illustrative studies                                                                                                                                                                                                                                                                                                                                                                                                                                       |
|-------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Phase I – Foundations and credible pilots (2026–2030) | Lays the groundwork for AI-driven integrated energy systems by hardening data infrastructure and demonstrating credible pilots at asset, building, district, and microgrid scales. Digital twins of buildings and local networks are used to coordinate PV, HVAC, storage, EV chargers, and demand response, mainly within single sectors or campuses. Early multi-energy hubs link electricity with heating/cooling and limited | Supervised learning, deep neural networks, and surrogate models dominate forecasting (loads, PV, prices, heat) and control, with early digital-twin platforms and rule-based / MPC controllers. Edge AI appears for device-level optimization and diagnostics, while explainable AI is piloted for asset health and operator trust. Blockchain and IoT platforms provide secure data streams, but integration across sectors is still partial. | Targets focus on demonstrable efficiency gains (5–25% energy savings), improved comfort and reliability, fault detection, and reduced O&M costs. Pilots show AI-enabled PV tracking, smart building control, and microgrid scheduling that cut peak demand and increase renewable hosting capacity, while building evidence on cyber-physical safety, validation of | Smart buildings and campuses with PV, batteries, and thermal storage; hydrogen refuelling and microgrids; small water–energy nexus facilities; EV charging hubs; industrial parks with AI-assisted process optimization. Use-cases include digital-twin-enabled building control, microgrid health management, PV cooling/dust mitigation, and hybrid hydrogen systems. | Priorities include: common data models and ontologies; open testbeds for buildings, microgrids, and hydrogen stations; standardized KPIs for AI-IES pilots; benchmarking of AI vs non-AI baselines; early cyber-security and privacy frameworks; and capacity-building in utilities and cities. Funding incentives encourage credible demonstration projects with rigorous M&V, especially in emerging economies. | Digital-twin buildings and residential hubs [4]; smart-building policy and socio-technical framing [138]; DT-driven microgrid health management [65]; ANN-based intelligent building PV cooling and dust control [201]; GAN-enhanced PV integration and robust operation [23]; AI-optimized geothermal–H <sub>2</sub> co-production [43]; AI-based micro-gas-turbine operation in microgrids [160]; AI-driven H <sub>2</sub> refuelling and hybrid systems |

|                                                                        |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |                                                                                                                                                                                                                                                                                                                              |                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |
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|                                                                        | gas, often in testbeds or smart districts rather than whole regions.                                                                                                                                                                                                                                                                                                                                                                                                                              |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | surrogates, and robustness under real-world uncertainty.                                                                                                                                                                                                                                                                                                                                                                                                                                                        |                                                                                                                                                                                                                                                                                                                              |                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | [3, 47].                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
| Phase II – Scaled, interoperable, and human-centric AI-IES (2030–2040) | Expands from pilots to city-, regional-, and national-scale integrated systems. Multi-vector infrastructures link electricity, gas, district heating/cooling, hydrogen, and mobility, orchestrated through interoperable platforms. Virtual power plants (VPPs), hybrid microgrids, and district-level energy hubs are co-optimized with water, waste, and mobility services. Human-centric design becomes central, coupling AI automation with operator oversight and citizen-facing interfaces. | Reinforcement learning (RL) and multi-agent RL coordinate DERs, EV fleets, storage, and flexible industrial loads. Hybrid physics-ML surrogates are embedded in planning and operations, with explainable AI for regulatory compliance and operator trust. Cross-sector digital twins (districts, industrial parks, ports) integrate IoT, edge/fog computing, and high-performance cloud analytics. Federated and distributed learning begin to address privacy and data-sovereignty constraints across utilities and regions. | Systems target high renewable shares (>70–90%), net-zero or net-negative emissions for specific clusters, and multi-objective optimization across cost, resilience, and societal acceptance. AI-IES manage flexibility markets, orchestrate V2G and smart EV charging, coordinate multi-carrier storage (batteries, hydrogen, thermal), and maintain power quality in high-PV grids. Resilience metrics (recovery time, service continuity) and sector-coupling indicators become routine performance criteria. | Regional multi-vector energy corridors; hydrogen and Power-to-X clusters; smart ports; industrial parks as “energy-materials-carbon” hubs; integrated EV-PV-BESS neighbourhoods; district heating networks coupled with heat pumps and thermal storage; water-resource recovery facilities optimized for energy circularity. | Priorities include: interoperability standards for data and control (across vectors and vendors); large-scale DT/VPP platforms; robust DRL/MARL safety and verification; socio-technical co-design with communities; integrated planning of energy–water–mobility; and cross-border market rules for flexibility and hydrogen trade. Regulatory sandboxes evolve into full-scale regulatory frameworks embedding AI ethics, transparency, and human-in-the-loop requirements. | Multi-vector coordination and techno-economic assessment for regional systems [2]; DRL-based multi-objective VPP and smart-grid optimization [112]; systematic review of hybrid HRES and sector-coupled systems [64]; AI-driven hybrid control in hydrogen-integrated microgrids with V2G [18]; EV-PV-BESS charging optimization in dense residential areas [90]; AI-driven industrial parks and mega-scale decarbonized petrochemical clusters [24]; AI-optimized energy-circular water resource recovery facilities [17]; district-scale hydrogen and ammonia SOFC plants with AI tri-objective optimization [62]; generative spatial AI for urban energy twins and smart cities [89]. |
| Phase III – Autonomous, resilient, and just AI-IES (2040–2050)         | Matures into globally networked, largely autonomous AI-IES that are deeply                                                                                                                                                                                                                                                                                                                                                                                                                        | Multi-agent RL ecosystems, neuromorphic and edge AI, and fully integrated digital twins                                                                                                                                                                                                                                                                                                                                                                                                                                        | Targets move beyond net-zero to net-negative emissions at system level, with strong                                                                                                                                                                                                                                                                                                                                                                                                                             | Planet-scale sensing and SAGIN-enabled control; AI-orchestrated supergrids and hydrogen                                                                                                                                                                                                                                      | Priorities centre on: formal verification and assurance of autonomous AI-IES; global governance for                                                                                                                                                                                                                                                                                                                                                                           | Integrated sensing-communication-computation architectures enabling wide-area                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |

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|  | entangled with urban form, critical infrastructure, and social systems. Cross-continental supergrids, hydrogen backbones, and space-air-ground integrated networks (SAGIN) support sector-coupled, climate-resilient energy services. Justice-oriented planning instruments ensure that AI-IES explicitly target energy poverty reduction, climate adaptation, and equitable access. | enable self-organising, self-healing infrastructures. Integrated sensing–communication–computation stacks feed high-fidelity twins of cities, grids, and industrial corridors, while physics-informed and constraint-aware learning enforce safety, stability, and climate constraints. Generative AI assists “design-to-policy” workflows, automatically proposing infrastructure reconfigurations, retrofits, and relocation strategies under deep uncertainty. | emphasis on climate resilience (heatwaves, floods, compound hazards), cyber-resilience, and social welfare metrics. AI-IES autonomously reconfigure networks, re-route power and fuels, adapt tariffs and incentives in real time, and proactively coordinate energy-water-food systems. Embedded justice metrics monitor distribution of benefits and burdens across regions and communities, guiding corrective interventions. | corridors; just-transition redevelopment of coal and gas regions; AI-driven smart irrigation and climate-resilient agri-energy landscapes; building and mobility systems that double as adaptive climate-risk buffers; water-energy-waste loops in circular, regenerative cities. | AI, data, and climate justice; mechanisms for participatory oversight and redress; integration of climate models and adaptation pathways into operational control; and capacity-building for regulators in low- and middle-income countries. Research pushes towards embedding ethics, explainability, and distributive justice into objective functions and constraints of AI controllers, making “just transition” a hard optimisation requirement rather than a narrative add-on. | autonomous operation [97]; 6G / SAGIN and multi-agent DRL frameworks for resilient task and resource allocation [136, 113, 151]; adaptive AI networks for ultra-efficient low-latency IoT in immersive environments [219]; justice- and policy-oriented energy planning for decarbonized cities and regions [168, 138, 102]; smart-irrigation and climate-resilient water–energy systems using AI and solar [122]; explainable AI for building-energy and GHG assessments [56]; AI-enabled energy-circular wastewater systems and bioenergy [83]; AI-integrated biomass-to-bioenergy and carbon-capture chains [139]. |
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## 9. Conclusions and Policy Recommendations

The analysis started by outlining a case for AI-Driven Integrated Energy Systems (AI-IES), contending that the non-linear dynamics, stochastic behaviour, and cross-sector couplings typical of multi-energy infrastructures are mounting challenges to traditional deterministic and scenario-based approaches. Machine learning, deep learning, reinforcement learning, physics-informed models, digital twins, and graph-based approaches are some of the techniques that can be systematically aligned with planning, operation, and control functions across electricity, heat, gas, hydrogen, and mobility networks. Artificial intelligence was not presented as a standalone forecasting tool.

The methodological framework then introduced a strict review procedure and classification schema. With extra tags for vector couplings, spatial scale, temporal horizon, performance objectives, and contextual setting, the literature was mapped onto a two-dimensional grid of AI method families and IES functions. From building and

district multi-energy hubs and community microgrids to regional multi-vector infrastructures, sector-coupled industrial clusters, and urban energy twins, this made it possible to compare system typologies and optimisation techniques in an organised manner.

Simultaneously, the synthesis revealed enduring deficiencies, such as inadequate integration of social and equity metrics into planning and operation, fragmented approaches to cyber-physical security, poor treatment of model drift and uncertainty, and limited validation of AI-IES models using actual operational data. A three-phase roadmap was put forth (2026–2030, 2030–2040, and 2040–2050), covering foundational benchmarks and pilots, scaled and interoperable deployments, and, in the end, autonomous but human-centred AI-IES that can degrade gracefully and quickly recover from compound shocks. The main conclusion is that while AI-IES are technically possible and are already showing promise in certain situations, their ability to support the global transition goals of 2030–2050 will rely more on the coherence of policy, governance, and market frameworks that influence the development, validation, and application of these tools than on discrete algorithmic advancements. Five strategic policy pillars are thus suggested to direct implementation.

### 9.1 Policy Pillar 1: Data, Digital Infrastructure, and Open Benchmarks

Strong digital foundations are the focus of the first pillar. Any AI-IES strategy is built on top of high-quality, granular data streams from smart grids, gas and heat networks, hydrogen assets, EV infrastructure, and industrial facilities. However, there are still many obstacles, such as fragmented data, inconsistent standards, and limited access. To encourage utilities, aggregators, and industrial actors to share anonymised, high-resolution datasets under explicit governance guidelines, policy frameworks should support interoperable data standards for multi-vector systems. It should be possible to compare AI techniques and hybrid models transparently by creating open benchmark repositories for multi-energy forecasting, dispatch, and resilience scenarios. Rather than being considered an auxiliary ICT layer, investments in safe, scalable digital infrastructure—such as edge computing, secure clouds, 5G/6G connectivity, and time-synchronized measurement systems—should be viewed as essential energy infrastructure.

### 9.2 Policy Pillar 2: Regulation, Standards, and Governance of AI in Critical Energy Systems

The regulatory and governance framework required for the secure, reliable integration of AI into vital energy infrastructure is covered in the second pillar. As learning-based controllers impact dispatch, market participation, and emergency response, AI-IES deployments raise concerns about algorithmic bias, safety, accountability, and dependability. Before AI agents are permitted to function in delicate decision loops, energy regulators and system operators demand precise requirements for model transparency, explainability, testing, and certification. With stringent oversight, regulatory sandboxes can offer safe spaces for testing AI-based tariffs, flexibility services, and automated market participation. Standards organisations should develop guidelines for acceptable autonomy levels, human-in-the-loop specifications, and fail-safe methods for multi-agent coordination and reinforcement learning.

### 9.3 Policy Pillar 3: Market Design and Investment Frameworks for Multi-Vector Flexibility and AI Services

This third pillar focuses on matching financing arrangements and price signals to the multi-vector flexibility and optimisation potential that artificial intelligence has produced. Cross-vector flexibility, resilience, and environmental co-benefits are frequently undervalued in current market designs, which favour single-vector optimisation and short-term cost minimisation. The establishment of multi-carrier flexibility markets and tariffs that incentivise the coordinated use of mobility assets, heat, gas, hydrogen, and electricity should be part of the reforms. To provide services like demand response, congestion management, and resilience enhancement, regulatory frameworks must permit aggregators and AI-enabled energy service providers to engage on an equal basis with more established players. The contribution of AI-optimized multi-vector assets, such as power-to-X facilities and storage systems, to system adequacy and emissions reduction must be reflected in long-term capacity and infrastructure compensation mechanisms. Targeting AI-IES demonstration projects in strategic locations such as ports, urban areas, industrial hubs, and cross-border corridors with public and blended finance can result in bankable reference cases that lower perceived risk and attract private investment. To unlock investment at scale, cost-benefit analyses and planning methodologies must explicitly acknowledge the benefits of AI-enabled systems. [199]

### 9.4 Policy Pillar 4: Capacity Building, Institutional Innovation, and Inclusive Participation

The fourth pillar acknowledges that technical sophistication is not enough on its own; institutional capacity and human skills are what determine whether AI-IES turn into transparent black boxes or reliable tools. Energy regulators, system operators, planners, municipal authorities, and community organisations need new skill sets in data analytics, AI governance, and socio-technical system design. Deployments of AI-IES may be resisted, abused, or underutilised in the absence of such capability. Therefore, interdisciplinary training programs that integrate power systems, gas and thermal engineering, artificial intelligence, cyber-security, and social sciences should be supported by policy initiatives. Smaller utilities and municipalities could benefit from shared analytical capabilities offered by regional centres of excellence in AI-IES. To break down silos between engineering, ICT, planning, and social policy, new organisational structures may be required at the institutional level. Examples include cross-departmental urban innovation units or specialised AI and digital twin teams within system operators. From the beginning, AI-IES projects should incorporate mechanisms for inclusive participation. Community, consumer, and civil society-based stakeholder engagement processes can help define acceptable trade-offs, address privacy or exclusion concerns, and guarantee that AI-enabled efficiency gains result in real benefits like increased comfort, affordability, and dependability.

### 9.5 Policy Pillar 5: International Cooperation and Just Transition Support

The last pillar places a strong emphasis on global collaboration and implementation that is focused on justice. AI-IES hold special promise in climate-vulnerable areas, island states, and emerging economies where decarbonisation, energy access, and resilience can all be advanced at the same time through integrated planning of renewables, storage, and flexible loads. Therefore, global policy frameworks should

support technology transfer, cooperative open-source tool development, and cooperative research initiatives that adapt AI-IES solutions to regional resource endowments, institutional realities, and cultural norms. AI-IES projects that clearly improve mitigation and adaptation outcomes can be given priority in climate finance and development assistance, with precautions taken to prevent inequality from getting worse. By facilitating the sharing of benchmark datasets, reference models, and best-practice case studies, multilateral platforms can guarantee that a wide range of nations and utilities can benefit from the lessons learnt by early adopters. With particular attention to the distributional effects of AI-IES deployment on employees, communities, and vulnerable groups, a just transition viewpoint should continue to be at the forefront. Targeted subsidies, social tariffs, and retraining programs are examples of policy tools that can help guarantee that the benefits are widely distributed and that the disruption of current livelihoods is handled equitably. Together, these five policy pillars offer a strategic framework for converting the technological potential of AI-driven integrated energy systems into tangible, fair advancements towards the global energy and climate goals of 2030–2050. AI-IES can transform from isolated pilots into a key enabler of just, resilient, and sustainable multi-energy infrastructures globally by combining methodological innovation with strong governance, market reform, capacity building, and international solidarity.

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## CONFLICTS OF INTEREST

The author declares that there is no conflict of interest regarding the publication of this paper

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