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Review Article

Ammonia splitting at the crossroads of advanced chemistry and industry 4.0/5.0

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Ammonia electrolysis offers an attractive alternative to conventional water electrolysis for sustainable hydrogen production, enabled by its lower theoretical energy requirement and established ammonia infrastructure. However, practical deployment remains constrained by the gap between laboratory catalyst performance and electrolyzer operation at industrially relevant current densities. This review critically examines ammonia electrolysis using an integrated framework that spans mechanistic catalyst design, device engineering, and Industry 4.0/5.0 concepts. Relationships among catalyst descriptors, reaction energetics, and electrochemical performance are discussed alongside challenges in electrode architecture, membrane electrode assemblies, and system integration. The roles of artificial intelligence, autonomous experimentation, and digital twins in accelerating catalyst discovery and predictive electrolyzer operation are evaluated, with emphasis on data quality, model reliability, and experimental validation. Integrating mechanistic insight, digital intelligence, and sustainable system design provides a roadmap toward scalable, low-carbon hydrogen production.

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Introduction: ammonia splitting at the chemistry digital interface

The transition toward a hydrogen-based energy economy requires cost-effective and energy-efficient hydrogen production technologies. To accelerate this goal, the U.S. Department of Energy's Hydrogen Shot initiative targets a production cost of US$1 kg^{-1} H_2 by 2031 [1]. Among the emerging alternatives to conventional water electrolysis, ammonia electrolysis has attracted increasing attention because ammonia combines a high hydrogen content (17.6 wt%), established production and distribution infrastructure, and a lower theoretical cell voltage, making it an attractive hydrogen carrier and feedstock for decentralized hydrogen production [2,3].

Despite its favorable thermodynamics, practical ammonia electrolysis remains far from industrial deployment. Practical performance is limited by sluggish ammonia oxidation kinetics, nitrogen poisoning, catalyst degradation, and system-level losses associated with electrode mismatch, membrane resistance, mass transport, and reactor architecture. Consequently, many catalysts that exhibit excellent activity under half-cell conditions (<10 mA cm^{-2}, short-term testing) fail to deliver comparable performance in practically relevant electrolyzers operating at high current densities (>100 mA cm^{-2}) [4,5]. This discrepancy highlights that catalyst activity alone cannot deliver practical ammonia electrolysis.

Most existing reviews focus on catalyst development, treating device engineering, digital optimization, and sustainability separately. However, successful commercialization requires these aspects to be considered as an integrated framework. This review, therefore, provides a critical perspective that connects mechanistic catalyst design with system-level engineering, Industry 4.0-enabled digital optimization, and Industry 5.0-driven sustainability. By identifying the factors limiting practical implementation, this review outlines a roadmap for translating ammonia electrolysis into scalable and sustainable hydrogen production.

Mechanistic chemistry and catalyst design principles

Electrochemical ammonia splitting is thermodynamically more favorable than water electrolysis, requiring a theoretical cell voltage of ~0.06 V compared with 1.23 V. However, practical operation requires 0.6–1.2 V at industrially relevant current densities (>100 mA cm^{-2}),

indicating that kinetic and transport losses dominate energy consumption. The ~0.06 V value represents the reversible thermodynamic cell potential and excludes kinetic overpotentials, ohmic resistance, mass-transport losses, membrane resistance, and auxiliary loads. Thus, the practical cell voltage of ~0.6−1.2 V at high current density represents a substantially different energy requirement; comparisons with water electrolysis should therefore use full-cell electrical consumption under defined operating conditions rather than theoretical voltage alone. The ammonia oxidation reaction (AOR) proceeds through a complex six-electron pathway involving multiple adsorbed nitrogen intermediates, while the hydrogen evolution reaction (HER) occurs at the cathode. Consequently, practical performance is governed primarily by reaction kinetics rather than thermodynamics [6].

Reaction pathways and mechanistic bottlenecks

Ammonia oxidation can involve sequential dehydrogenation of adsorbed NH_3 via NH_x intermediates, followed by N−N bond formation and desorption of nitrogen-containing products; however, the dominant pathway strongly depends on catalyst composition and surface structure. Different NH_x intermediates may participate in N−N coupling, while strongly adsorbed N can instead accumulate on active sites and promote catalyst poisoning. Thus, the commonly depicted $NH_3 \rightarrow NH_2^* \rightarrow NH^* \rightarrow N^*$ sequence should be regarded as a simplified mechanistic framework rather than a universal pathway.

Recent theoretical and operando studies indicate that the rate-determining step depends on catalyst composition and surface structure [4]. On Ni-based catalysts, electrochemical reconstruction to NiOOH promotes ammonia activation but also increases susceptibility to nitrogen accumulation during prolonged operation [7]. Alloying and heterostructure formation modify the electronic environment of active sites, lowering intermediate-conversion barriers while improving catalyst stability. Overall, catalytic performance depends on balancing ammonia activation, intermediate conversion, and nitrogen removal [8].

Mechanistic descriptors for rational catalyst design

Catalyst development has evolved from empirical material screening to descriptor-based design, where catalytic performance is correlated with electronic structure rather than composition alone. Key descriptors include the adsorption free energies of the NH_x and N* intermediates, the d-band center, the hydroxyl adsorption energy, and the charge-transfer characteristics, which collectively govern activity, selectivity, and resistance to nitrogen poisoning. Electronic structure engineering through alloying, defect creation, heterointerfaces, and single-atom catalysts optimizes these descriptors by balancing intermediate adsorption and desorption, thereby accelerating the multi-step AOR pathway while improving catalyst stability [9,10]. Because adsorption energies of NH_x and N-containing intermediates are often correlated through scaling relationships, independently optimizing each intermediate is difficult; therefore, catalyst design increasingly seeks to modify local coordination, alloy composition, or interfaces to partially decouple this energetics.

From catalyst activity to practical electrolysis

Despite remarkable advances in catalyst design, improvements in intrinsic activity have translated only modestly into practical electrolyzer performance. Most catalysts are evaluated under half-cell conditions at low current densities and short operating durations, where limitations associated with electrode architecture, mass transport, membrane resistance, and catalyst utilization are largely absent. Consequently, catalysts demonstrating excellent laboratory performance frequently exhibit substantial voltage losses and accelerated degradation under industrially relevant conditions. This disparity highlights that catalyst optimization alone is insufficient for practical ammonia electrolysis [11]. Future progress, therefore, depends on integrating mechanistic catalyst design with electrode engineering, reactor architecture, and operando diagnostics under realistic operating conditions.

Device engineering: bridging catalyst activity and practical ammonia electrolysis

Despite remarkable advances in catalyst development, improvements in intrinsic ammonia oxidation activity have translated only modestly into practical electrolyzer performance. This disparity reflects a fundamental limitation of current research: most catalysts are evaluated in three-electrode half-cell configurations under low current densities (<10 mA cm^{-2}), where intrinsic kinetics dominate and engineering constraints are largely absent. In contrast, practical ammonia electrolyzers operate at current densities exceeding 100 mA cm^{-2}, where electrode architecture, membrane properties, reactant transport, and current distribution become equally important determinants of efficiency. Consequently, catalyst performance cannot be evaluated independently of device design [11].

A major challenge is *balancing the ammonia oxidation reaction (AOR) with the hydrogen evolution reaction (HER).* While catalyst development has focused predominantly on improving anodic AOR activity, the cathode is often treated as non-limiting. This assumption frequently results in polarization mismatch, higher cell voltages, and reduced energy efficiency. Future catalyst development should therefore prioritize electrode compatibility and full-cell optimization rather than maximizing isolated half-cell activity [8,9].

Mass transport presents another major bottleneck under practical operating conditions. Ammonia depletion near the anode, nitrogen bubble accumulation, and concentration polarization progressively reduce catalyst utilization despite high intrinsic activity. Although porous electrodes, hierarchical architectures, and flow-through electrolyzers improve reactant delivery and gas removal, their influence on long-term durability and industrial operation remains insufficiently investigated [11,12].

Similarly, *membrane development* has received considerably less attention than catalyst design, despite its central role in practical ammonia electrolysis. Membranes must simultaneously provide high ionic conductivity while suppressing ammonia crossover, which lowers Faradaic efficiency, alters cathodic reaction environments, and accelerates degradation [11–13]. However, systematic studies correlating membrane properties with long-term electrolyzer performance remain scarce.

The transition from laboratory cells to membrane electrode assemblies (MEAs) and stack-level systems introduces additional challenges that are rarely captured in half-cell studies. Non-uniform current distribution, thermal gradients, interfacial resistance, and uneven reactant flow create localized degradation and reduce overall system efficiency. Although recent MEA studies demonstrate that flow-field geometry, electrode compression, and electrolyte management strongly influence performance, experimental validation under industrially relevant operating conditions remains limited, with most studies still confined to laboratory-scale H-cell configurations [6,11,12].

Collectively, these observations indicate that the principal barrier to commercialization is no longer catalyst discovery alone but the absence of integrated device engineering. Accordingly, practical energy consumption should be evaluated based on the operating cell voltage and current required to produce a quantified hydrogen output, while explicitly distinguishing stack-level electrical demand from auxiliary loads such as pumping, gas separation, and thermal management.

Industry 4.0: digital acceleration of ammonia splitting

Industry 4.0 refers to the digital transformation of manufacturing through artificial intelligence (AI), machine learning (ML), automation, robotics, the Internet of Things (IoT), cloud computing, and digital twins. For ammonia electrolysis, these technologies offer opportunities beyond catalyst screening by simultaneously optimizing catalyst properties, device architecture, operating conditions, and long-term performance. Importantly, the level of maturity differs among these approaches: data-driven catalyst analysis and automated electrochemical measurements have been demonstrated in related electrochemical systems, whereas integrated autonomous experimentation, real-time digital twins, and closed-loop process control remain largely prospective for ammonia electrolysis. Their translation to ammonia systems is constrained by limited standardized datasets and scarce industrial-scale validation.

AI-assisted catalyst discovery and autonomous experimentation

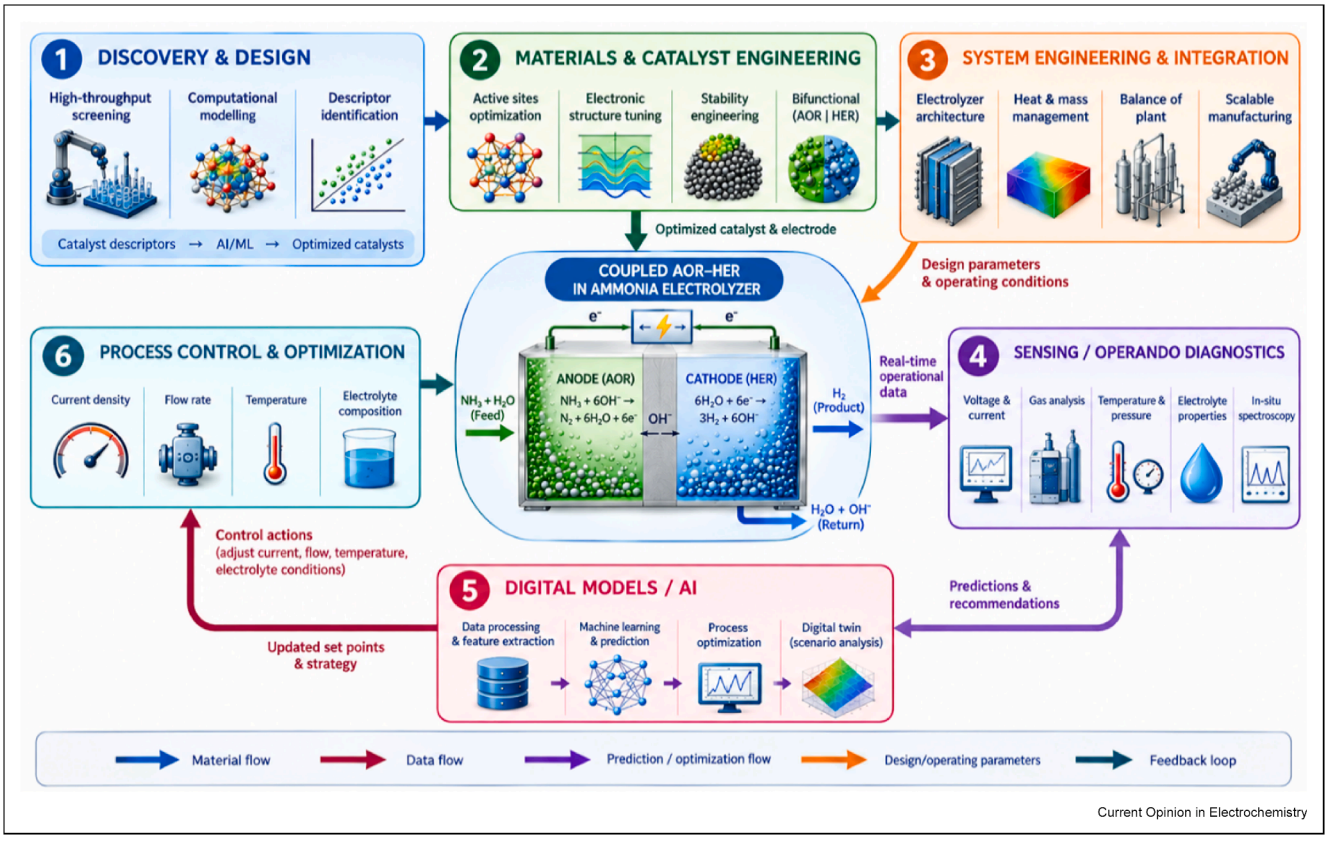
AI and ML have shifted catalyst development from empirical screening toward descriptor-based optimization. For ammonia oxidation, descriptors such as NH_3/NH_x adsorption energies, nitrogen binding energy (ΔG_{N^*}), d-band center, hydroxyl adsorption energy, and charge-transfer characteristics govern catalyst activity, selectivity, and resistance to nitrogen poisoning. Integrating these descriptors with density functional theory (DFT), operando characterization, and experimental polarization data enables rapid identification of promising catalyst compositions while optimizing electrolyte composition, ammonia concentration, operating potential, and temperature. However, ammonia-specific datasets suitable for robust machine-learning training remain scarce and fragmented, with limited combinations of catalyst descriptors, standardized AOR performance, Faradaic efficiency, and long-term durability data. This scarcity, together with inconsistent protocols, restricts model transferability across catalyst systems.

In principle, automation could complement AI by generating reproducible datasets through robotic synthesis and high-throughput electrochemical testing; however, such closed-loop workflows remain largely prospective for ammonia electrolysis. When coupled with operando techniques such as impedance spectroscopy, Raman spectroscopy, differential electrochemical mass spectrometry, and online gas analysis, autonomous platforms enable continuous monitoring of catalyst reconstruction, nitrogen poisoning, electrolyte degradation, and reaction selectivity. Beyond accelerating catalyst discovery, these closed-loop workflows improve benchmarking consistency and provide the high-quality experimental data required for robust machine-learning models [14–17].

Digital twins for intelligent ammonia electrolyzers

Digital twins can extend digital optimization from catalyst discovery to device operation by integrating electrochemical kinetics, mass transport, and reactor engineering into predictive virtual models. While digital-twin implementations have been demonstrated for PEM electrolyzers and integrated hydrogen-energy systems, their application to ammonia electrolysis remains largely prospective and requires ammonia-specific validation (Figure 1). Real-time sensor data, including cell voltage, impedance, ammonia concentration, gas

Figure 1



Integrated research and scale-up framework for coupled AOR–HER ammonia electrolysis, illustrating the flow of material, experimental data, digital prediction, and feedback control.

evolution, electrolyte conductivity, flow rate, and temperature, enable continuous prediction of ammonia crossover, nitrogen bubble accumulation, catalyst degradation, membrane ageing, concentration polarization, and non-uniform current distribution before substantial performance losses occur. These measurements can form a closed feedback loop in which sensed electrolyzer states update the digital model, model predictions identify deviations or optimal operating conditions, and control actions adjust current, flow, temperature, or electrolyte conditions in the physical electrolyzer. Such models facilitate virtual optimization of flow-field geometry, electrode compression, stack configuration, and operating strategies, reducing the cost and time required for scale-up.

Despite these opportunities, digital implementation in ammonia electrolysis remains considerably less mature than in water electrolysis or battery systems. Most reported studies rely on simplified laboratory-scale models with limited experimental validation, highlighting the need for integrated electrochemical, transport, and operational datasets. Consequently, the future impact of Industry 4.0 will depend not only on advances in AI algorithms but also on establishing standardized experimental protocols and interoperable data platforms that connect catalyst design, device engineering, and real-time electrolyzer operation [18–20].

From industry 4.0 to industry 5.0: sustainability and human-centric scaling

While Industry 4.0 focuses on digitalization, automation, and data-driven optimization, Industry 5.0 extends these concepts by emphasizing sustainability, resilience, safety, and human-centered decision-making. For ammonia electrolysis, this shift is particularly important because commercialization depends not only on performance but also on safe handling of ammonia, environmental sustainability, and economic viability.

Industry 5.0, therefore, integrates renewable electricity, green ammonia production, circular catalyst manufacturing, life-cycle assessment (LCA) [21], and techno-economic analysis (TEA) into electrolyzer development. Intelligent monitoring systems capable of detecting ammonia leakage, hydrogen accumulation,

and abnormal operating conditions can improve operational safety, while human expertise remains essential for interpreting AI predictions and validating autonomous decisions. By combining digital intelligence with responsible process design, Industry 5.0 provides a framework for developing ammonia electrolyzers that are not only efficient but also safe, resilient, and environmentally sustainable [1,22].

Future perspectives and outlook

The future of ammonia electrolysis depends on shifting from catalyst-centered research toward integrated electrochemical system design. Progress will require standardized benchmarking protocols, long-term validation under industrially relevant conditions, and co-optimization of catalysts, membranes, electrodes, and reactor architecture. Equally important is the development of interoperable datasets that combine catalyst descriptors, operando characterization, and device-level performance to support reliable AI models and digital twins.

Beyond improving efficiency, future ammonia electrolyzers must also satisfy the broader objectives of Industry 5.0 by integrating renewable electricity, green ammonia, circular materials, intelligent safety systems, and techno-economic assessment into practical device development. Bridging mechanistic chemistry, engineering, and digital intelligence will be essential to translating laboratory discoveries into scalable, low-carbon hydrogen production.

CRediT authorship contribution statement

Anit Joseph: Conceptualization, Validation, Writing-original draft. **Tiju Thomas**: Supervision, Conceptualization, Validation, Writing-review & editing.

Generative AI

We acknowledge that AI-assisted graphical generation was used during the preparation of certain visual elements of Figure 1. The scientific content, organization, interpretation, and final assembly of the figure were determined and verified by the authors. The authors used AI-assisted tools (ChatGPT, Perplexity, and Grammarly) solely for language editing and clarity, and take full responsibility for the content of the manuscript.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Data availability

Data will be made available on request.

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