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Degradation of Electrochemical Materials in Energy Conversion and Storage

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Electrochemical materials are the cornerstones of next-generation energy technologies, from high-energy-density batteries and fuel cells to green hydrogen electrolyzers. While a lot of research has focused on maximizing the initial functional metrics of these materials, the focus is rapidly shifting toward structural and electrochemical durability. Degradation is not merely a loss of performance; it represents a fundamental, often irreversible, evolution of the material's identity under the harsh conditions of device operation. Consequently, recent years have witnessed a surge in research dedicated to deciphering the intrinsic coupling between functional activity and degradation/corrosion mechanisms. By leveraging synergistic breakthroughs in high-resolution *in situ* characterization and high-fidelity computational modeling, we can now resolve these degradation pathways with unprecedented mechanistic clarity.

This special issue, "Degradation of Electrochemical Materials in Energy Conversion and Storage," explores the complex interplay between material performance and stability. The contributions gathered here span a diverse spectrum of theoretical, computational, and experimental studies, aimed at bridging the gap between material behavior and long-term system longevity.

In the field of electrocatalysis, deciphering the mechanistic origins of the activity-stability trade-off remains one of the most critical and challenging frontiers of research. This relationship is rarely a simple correlation; rather, it is a complex competition where the highly reactive surface sites required to drive demanding reactions are often the most susceptible to structural disintegration or material dissolution. Transitioning from empirical trial-and-error catalyst synthesis to rational, stability-by-design strategies requires a rigorous understanding of these processes at the atomic scale. Li et al. computationally investigated activity-stability relationships in strain-engineered Pt-based oxygen reduction catalysts demonstrating that compressive strain optimizes *O binding for improved activity but this destabilizes the surface through reconstruction (10.1021/acs.jpcc.5c03738). Exner and coauthors assessed the thermodynamic stability of the single-atom catalyst (SAC)-like motifs of MXenes under anodic polarization OER conditions using density functional theory (DFT) calculations (10.1021/acs.jpcc.5c01252). Bolarin et al. employed statistical analysis through a factorial design of experiments (DoE) approach to examine the combined effects of different experimental parameters such as iridium thickness, titanium adhesion layer thickness and annealing temperature on the performance of sputtered iridium electrocatalysts in sulfuric acid (10.1021/acs.jpcc.5c03764). The process of cathodic corrosion on platinum electrodes in aqueous environments was analyzed by Koper and coauthors by means of ex situ microscopy showing that cathodic corrosion pits follow a nucleation-and-growth process (10.1021/acs.jpcc.5c05071). In the paper by Song et al. on the electrochemical nitrogen reduction, the coupling between surface oxygen vacancy configurations and the catalytic activity/structural stability of β-MoO_3 were investigated using first-principles DFT simulations (10.1021/acs.jpcc.5c03948). Jacob and coauthors also employed DFT calculations to study the nitrogen reduction reaction on Cu oxide-based electrocatalysts providing insights into preferential reaction sites, thermodynamic feasibility, and the overall reaction mechanisms (10.1021/acs.jpcc.5c03667).

In the realm of rechargeable batteries, the longevity and power density of the system are largely dictated by the physicochemical evolution of their interfaces. Central to this is the formation and growth of the solid electrolyte interphase (SEI)—a complex, multicomponent passivation layer that forms on the anode during the initial cycles. The contributions in this section utilized advanced computational and experimental methods to examine interfacial evolution providing a path toward predictive battery design. For example, Guerrero-Navarro et al. carried out a theoretical/computational analysis of the SEI growth and degradation dynamics occurring in lithium metal batteries during cycling (10.1021/acs.jpcc.5c04292). Persson and coauthors employed an integrated framework based on high-throughput first-principles calculations and machine learning interatomic potentials to explore interphase formation between lithium metal anodes and an inorganic solid-state electrolyte (10.1021/acs.jpcc.5c03589). Bar-lev et al. applied electrochemical and

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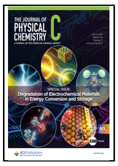

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structural analyses to investigate the degradation mechanisms of poly(ethylene oxide)-based solid polymer electrolytes (SPEs) paired with Li nickel manganese cobalt oxide (NMC) cathodes (10.1021/acs.jpcc.5c03533).

While the rapid rise in power conversion efficiency for emerging photovoltaics has been remarkable, the path to commercialization is currently hampered by the intrinsic and extrinsic instability of the active materials. In contrast to traditional silicon-based devices, next-generation optoelectronic materials such as halide perovskites and organic semiconductors exhibit a soft, dynamic lattice that is highly sensitive to environmental factors. For instance, Miyazawa et al. performed in situ evaluation of organohalide perovskite solar cells under proton irradiation at low temperatures representative of the space environment (10.1021/acs.jpcc.5c02899). The role of device voltage as a contributor to organic semiconductor degradation was studied using IR reflectance−absorbance spectroscopy and X-ray photoelectron spectroscopy by Pemberton and coauthors (10.1021/acs.jpcc.5c05633).

The investigation of complex degradation phenomena across different electrochemical energy systems is supported by a suite of cutting-edge methodological contributions. The group led by Moreno-Hernandez highlighted the transformative role of in situ electrochemical liquid-phase transmission electron microscopy (LP-TEM) (10.1021/acs.jpcc.5c01320). This technique serves as a “nanoscopic window”, enabling the acquisition of high-resolution image series under operational bias to directly visualize the real-time morphological evolution and dissolution of electrochemical materials. Reese et al. demonstrated the power of electrochemical atomic force microscopy (EC-AFM) in providing unprecedented insights into the microstructure of electrode−electrolyte interfaces during electrochemical reactions (10.1021/acs.jpcc.4c08291). Beyond characterization, the ability to synthesize and process materials under extreme conditions offers new pathways to stability. Gottesman contributed a Perspective on the use of physical vapor deposition coupled with rapid photonic annealing (10.1021/acs.jpcc.5c04338). This method achieves ultrafast heating rates (10^2−10^7 K/s), far exceeding the limits of conventional conduction or convection (~0.01−1 K/s). Such thermal nonequilibrium conditions facilitate high-temperature crystallization while preserving substrate integrity. Leung provided an insightful computational Perspective article discussing the principles of electronic structure modeling of battery interfaces (10.1021/acs.jpcc.5c00616).

This special issue also features a Review article by Bandarenka and coauthors on degradation mechanisms of Prussian Blue Analogues and state-of-the-art approaches to stability optimization (10.1021/acs.jpcc.5c00877). The authors discuss the impact of transition metal dissolution, phase transitions, the Jahn−Teller effect, crystal defects, coordinated water, side reactions, and other degradation mechanisms.

In summary, the contributions within this special issues underscore a pivotal shift in the field: the transition from empirical observation to a predictive, stability-centric paradigm in energy materials design. By integrating high-fidelity computational modeling with multimodal *in situ* characterization, we are finally bridging the gap between material functionality and longevity. This progress highlights the fundamental necessity of resolving atomic-scale mechanisms to accurately predict and control device performance.

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