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Editorial: Multiphysics, multiphase and multiscale modeling and characterization of porous media in electrochemical energy systems

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Editorial on the Research Topic
Multiphysics, multiphase and multiscale modeling and characterization of porous media in electrochemical energy systems

1 Introduction

Porous materials play an important role in the electrodes of electrochemical energy systems (e.g., fuel cells, batteries, and supercapacitors) by enhancing ion transport, increasing surface active area, and improving charge storage capacity. Porosity increases volumetric density of actives sites, allows efficient electrolyte penetration, facilitating fast ion diffusion and reducing resistance. In supercapacitors and batteries, materials like metal-organic frameworks, porous carbons, and mesoporous oxides improve energy density and cycle stability. They enable high-performance electrodes with superior conductivity and electrochemical stability. Additionally, tunable pore structures optimize ion accessibility, enhancing power output and charge-discharge efficiency. As energy demands grow, porous materials drive advancements in next-generation energy storage technologies, making them vital for sustainable energy solutions.

The optimal design of porous media in electrochemical energy systems poses fundamental questions due to the existence of conflicting effects in the desired effective properties (e.g., diffusivity, permeability, Young's modulus and electrical/thermal conductivity). Additionally, determining the optimal distribution of these effective transport properties to maximize performance and durability remains an open question. The complexity is further compounded by the multiscale nature of the problem, spanning from nanometers to centimeters within a single cell and beyond in cell stacks. Moreover, finite-size features, such as manufacturing defects, heterogeneous, multi-component microstructure and lack of a representative elementary volume across the thickness, complicate modeling and characterization efforts. Multiphase transport of either products or trapped secondary phases plays also a key role at different spatial and temporal scales, affecting reactant distribution, peak power density, efficiency and degradation.

This Research Topic aims to serve as a gathering point for researchers engaged in the modeling and characterization of electrochemical systems, emphasizing multiphysics, multiphase, and multiscale transport phenomena. The design of engineered porous media with enhanced properties is of paramount importance to improve performance and enlarge durability, while reducing cost and extending commercialization of electrochemical energy devices. Extraction of good guidelines to produce novel multifunctional porous media is essential as part of the design of next-generation electrochemical systems. Porous media of interest include but are not limited to transport porous layers, catalyst layers, macroporous electrodes, membranes and porous flow distributors.

2 Fuel cells

García-Salaberri et al. examine the origin, dependency and mitigation strategies of local oxygen transport resistance for the design of next-generation polymer electrolyte fuel cells (PEMFCs). They conclude that performance and durability targets set for the catalyst layer can be reached in the near term by using advanced catalyst layer preparation techniques (e.g., electrospraying) and the development of new materials with tailored properties (e.g., porous ionomers). Similarly, East et al. provide a comprehensive review of the performance of PEMFCs operated with ionic liquids as electrolytes. They identify three main limitations contributing to the reduced performance of PEMFCs with ionic liquid-holding membranes: poor conductivity, poor oxygen reduction kinetics, and seepage of the liquid from the membrane. The authors discuss recent advances made in the field over the past 5 years aimed at overcoming these drawbacks.

3 Batteries

Guo et al. examine the challenges and opportunities of aqueous Zn–CO_2 batteries, with a focus on the cathode catalysts. These batteries convert CO_2 into electricity while utilizing zinc, an abundant and recyclable material. By reducing atmospheric CO_2, these batteries contribute to climate change mitigation. Their low cost, sustainability, and scalability make them a viable alternative to lithium-ion batteries. In their paper, Guo et al. discuss design strategies and preparation methods for the development of efficient cathode catalysts (structure, charge distribution, and coordination environment). By advocating for the implementation of sound design practices rooted in fundamental principles, the authors envision a pathway towards the development of not only environmentally friendly but also high-performance energy storage systems capable of meeting the demands of tomorrow's energy landscape.

4 Supercapacitors

Lv et al. examine recent developments in supercapacitor electrodes made from carbonaceous materials, including their working principle, electrochemical parameters and preparation methods. The authors highlight the imperative for continued efforts towards surface modification and doping techniques to elevate the energy density of active carbon-based electrodes. Specifically, future work should be focused on waste residues derived from carbonaceous materials and scaled production processes that are in line with green energy policies.

5 Conclusion

Four review articles devoted to the modeling and characterization of innovative porous media for electrochemical applications were presented in this Research Topic. The work focused on the design and optimization of porous media and cutting-edge strategies to improve the operation of fuel cells, batteries and supercapacitors. The contributions provide a valuable piece of work to manufacturing techniques, transport in multifunctional porous media, such as catalyst layers and membranes, and performance and durability improvement. This collective body of work not only deepens our understanding of the intricate dynamics governing electrochemical systems but also paves the way for the development of more efficient and durable energy storage and conversion devices.

Author contributions

PG-S: Conceptualization, Formal Analysis, Funding acquisition, Investigation, Methodology, Project administration, Resources, Supervision, Writing – original draft, Writing – review and editing. AC: Formal Analysis, Funding acquisition, Investigation, Methodology, Writing – original draft, Writing – review and editing. PD: Formal Analysis, Investigation, Methodology, Writing – original draft, Writing – review and editing. MA: Formal Analysis, Investigation, Methodology, Writing – original draft, Writing – review and editing.

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Conflict of interest

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