Special Issue

Integration of Machine Learning and Modeling in Catalysis

Message from the Guest Editor

This special issue delves into the vital realm of solid-state electrolytes (SSE) in the development of energy storage solutions. It seeks to investigate the role of interpretable machine learning (ML) in the design and optimization of SSE materials. The background lies in the challenges faced in identifying commercially viable solid electrolytes, emphasizing the critical need for innovative approaches in this rapidly evolving field. The scope includes exploring ML algorithms for modeling solid-state electrolytes based on limited data, utilizing various databases to construct interpretable ML models specifically for solid-state ion batteries. This issue aims to enhance the understanding of material properties and facilitate targeted design and performance prediction of solid electrolytes. By integrating first-principles calculations to establish a high-quality testing database, this research aspires to accelerate the discovery of new materials, reduce R&D costs and timelines, and improve production efficiency. Ultimately, it contributes to the advancement of sustainable energy solutions, driving innovation in the field of solid-state electrolytes.

Guest Editor

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