Special Issue

Predictive Modeling in Catalysis

Message from the Guest Editor

Accurate prediction of catalytic performance—including activity, selectivity, and stability—is the cornerstone of rational catalyst design. This SI focuses on realistic and robust modeling strategies that bridge theory and experiment to enable predictive insights into both heterogeneous and molecule-based catalytic systems. We welcome contributions that employ a range of methodologies of different natures and scales, including quantum mechanical calculations, statistical mechanics, and data-driven approaches, with a balance of mechanistic insights and designs that leverage current knowledge. Emphasis is placed on models that go beyond simplistic or idealized systems to capture complex catalytic environments and phenomena, offering predictive power across reaction conditions, time and size scales, and material classes. We especially encourage approaches that challenge the status. By highlighting the advances in predictive models, this collection aims to advance the state-of-the-art in computational catalysis, connect the worlds of experiments and theories, and accelerate the discovery and optimization of practical catalytic systems.

Guest Editor

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