Special Issue

Catalysis at the Nanoscale: Insights from Theory and Simulation

Message from the Guest Editor

Catalysis lies at the heart of sustainable energy conversion, environmental remediation, and chemical synthesis. At the nanoscale, catalytic processes exhibit unique behaviors governed by quantum effects, surface dynamics, and atomistic interactions, which challenge conventional experimental characterization. Advances in theoretical modeling and computational simulations have emerged as indispensable tools to unravel these complexities, offering mechanistic insights and predictive power for designing next-generation catalysts. This Special Issue focuses on cutting-edge research at the intersection of nanoscience, catalysis, and computational methodologies. We invite contributions that explore topics such as (1) multiscale modeling of catalytic active sites, (2) machine learning-driven catalyst discovery, (3) reaction pathway analysis under realistic conditions, (4) dynamic evolution of nanostructures during catalysis, and (5) synergy between simulations and in situ/operando experiments. Submissions may address heterogeneous, homogeneous, or enzymatic systems, with an emphasis on energy-related applications.

Guest Editor

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Nanoscience and nanotechnology are exciting fields of research and development, with wide applications to electronic, optical, and magnetic devices, biology, medicine, energy, and defense. At the heart of these fields are the synthesis, characterization, modeling, and applications of new materials with lower nanometer-scale dimensions, which we call “nanomaterials”. These materials can exhibit unusual mesoscopic properties and include nanoparticles, coatings and thin films, metal–organic frameworks, membranes, nano-alloys, quantum dots, self-assemblies, 2D materials such as graphene, and nanotubes. Our journal, *Nanomaterials*, has the goal of publishing the highest quality papers on all aspects of nanomaterial science to an interdisciplinary scientific audience. All of our articles are published with rigorous refereeing and open access.

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