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Molecular Scale Studies of Computational Catalysis and Density Functional Theory in Materials Chemistry

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Message from the Guest Editor

Computational catalysis is an outstanding branch of science that merges different approaches to microkinetic modeling, atomistic simulations, and catalyst design based on fundamental concepts. Density functional theory (DFT), the work horse of atomistic simulation, and the variety of versions of DFT make it useful in both homogeneous and heterogeneous catalysis and allows it to be a successful tool of computational materials chemistry.

This Special Issue is mainly focused on computational catalysis and density functional theory in materials chemistry at the molecular scale, which involves predicting the structure and properties of molecules. By optimizing the geometric configuration of the molecule, its equilibrium structure can be obtained, thus allowing the vibration frequency, infrared spectrum, etc., of the molecule to be calculated. In addition, by calculating molecule properties such as electron affinity and ionization potential, the chemical reactivity and stability of molecules can be predicted, providing strong support for drug design and catalytic reaction mechanism research.

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Message from the Editor-in-Chief

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