Special Issue

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

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.

Guest Editor

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The International Journal of Molecular Sciences (*IJMS*, ISSN 1422-0067) is an open access journal, which was established in 2000. The journal aims to provide a forum for scholarly research on a range of topics, including biochemistry, molecular and cell biology, molecular biophysics, molecular medicine, and all aspects of molecular research in chemistry. *IJMS* publishes both original research and review articles, and regularly publishes special issues to highlight advances at the cutting edge of research. We invite you to read recent articles published in *IJMS* and consider publishing your next paper with us.

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