Special Issue

Modeling and Simulation of Next-Generation Catalytic Materials for Energy and Environment Applications

Message from the Guest Editors

In recent years, catalytic materials have played an increasingly pivotal role in driving innovations within the energy and environment sectors, particularly in the realms of industrial catalysis and fuel cell technology. These advances have been instrumental in pushing the boundaries of sustainability and efficiency. However, the complexity of these materials necessitates enhanced computational tools to fully comprehend their behavior and optimize their performance. This Special Issue, titled "Modeling and Simulation of Next-Generation Catalytic Materials for Energy and Environment Applications", seeks to highlight the leading computational methodologies being applied to the study of catalytic materials designed for energy and environment related applications. The aim is to bring together cutting-edge research that utilizes state-of-the-art computational tools such as density functional theory (DFT), molecular dynamics (MD), Monte Carlo (MC) simulations, and numerical modeling to explore the fundamental aspects of catalytic processes and material design.

Guest Editors

Dr. Houyu Zhu

Shandong Key Laboratory of Intelligent Energy Materials, School of Materials Science and Engineering, China University of Petroleum (East China), Qingdao 266580, China

Dr. Lianming Zhao

Shandong Key Laboratory of Intelligent Energy Materials, School of Materials Science and Engineering, China University of Petroleum (East China), Qingdao 266580, China

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Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland
Tel: +41 61 683 77 34
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Prof. Dr. Keith Hohn
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