Latest Advances in Molecular Modeling Applied in Chemical Processes

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Message from the Guest Editor

Dear Colleagues,

Understanding chemical processes is often only possible by revealing the molecular interactions at an atomic or even at an electronic level. Therefore, molecular modeling and simulation play an important role in analyzing chemical processes. The efficient identification of reaction pathways and reaction rates using advanced computational modeling and methods is an important aspect of this Special Issue. The complexity of pure ab initio calculations often prohibits the analysis of large molecular systems. Advances in this area of research are welcomed. However, complexity reduction, classical enhanced dynamical simulations, machine learning, and surrogate models are also modern approaches to overcome this hurdle and are part of the latest advances to be addressed.

Keywords

- machine learning
- model extraction
- surrogate model reaction
- pathways cascades of timescales

Special Issue

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Message from the Editor-in-Chief

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