Special Issue

Latest Advances in Molecular Modeling Applied in Chemical Processes

Message from the Guest Editor

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

Guest Editor

Dr. Weber Marcus

Zuse Institute Berlin (ZIB), Takustrasse 7, 14195 Berlin, Germany

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Processes
Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland
Tel: +41 61 683 77 34
processes@mdpi.com

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Editor-in-Chief

Prof. Dr. Giancarlo Cravotto
Department of Drug Science and Technology, University of Turin, Via P. Giuria 9, 10125 Turin, Italy

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