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Special Issue Reprint

Advances in Molecular Modeling in Chemistry, 2nd Edition

Edited by: Heng Zhang and Shiling Yuan

Molecular modeling has revolutionized the ways in which we understand, predict, and manipulate chemical systems, from simple molecules to complex biological macromaterials and functional nanomaterials. By bridging theory and experiment, computational approaches provide unprecedented insights into atomic-scale interactions, reaction mechanisms, and material properties, accelerating discovery across chemistry, biochemistry, and materials science.

This Reprint of the Special Issue entitled “Advances in Molecular Modeling in Chemistry” aims to showcase cutting-edge developments in computational chemistry and molecular simulation. The Special Issue highlights innovative methodologies, algorithms, and applications in areas such as quantum chemical calculations, molecular dynamics and Monte Carlo simulations, machine learning and artificial intelligence in chemical modeling, etc. The studies published within this Reprint explore areas such as molecular dynamics simulations of oil adsorption behavior, the antifoaming mechanisms of surfactants, density functional theory calculations of catalytic mechanisms, drug discovery, and the evaluation of combustion mechanisms using reactive molecule force fields, among other topics.

By bringing together diverse expertise, this Special Issue seeks to foster interdisciplinary dialog and inspire the next generation of computational strategies.

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