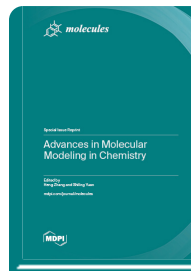


*Special Issue Reprint*

## Advances in Molecular Modeling in Chemistry

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Molecular modeling is playing a crucial role in chemistry investigations. With the current developments in computing power, it is possible to achieve large-scale simulations. Molecular modeling has been applied successfully in many areas of chemistry, e.g., the behavior of liquid solutions, proteins, DNA, polysaccharides, lipid membranes, crystals, amorphous solids, or any combination of them; the process of adsorption or desorption at interfaces; protein folding; self-assembly; etc.

Aside from the widely spread application of molecular modeling, the techniques of simulation also developed rapidly. Many simulation techniques have emerged, including ab initio molecular dynamics, polarizable force field, reactive molecular dynamics, machine learning accelerated simulation, metadynamics, etc.

This reprint includes 13 original papers reporting on molecular simulation works, including quantum chemistry calculation, molecular dynamic simulation, etc., or combined experiments and simulation studies. We hope that this collection of research studies can bring inspiration to readers regarding the application of molecular modeling methods.

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