

## Usage of Molecular Modeling and Simulation in Chemical Engineering

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Advances in molecular modeling and simulation have made great impacts on almost all research fields due to their well-defined ability to describe atomistic and molecular behaviors controlling macroscopic phenomena. Furthermore, the increase of the computer technology complementarily fulfills its implementations further into the topics that have never been dreamed to work on 30 some years ago. Those are typically nano- and biomaterials and their related systems in the chemical engineering field. As artificial exploration into atomistic world became possible via simulations developed over last decades, the research trend, which has been experiment-orientated, currently moves to greet the collaborative effort with computational study. The talk is particularly prepared to present various topics to show how impactful the interdisciplinary effort of molecular modeling and simulation and chemical engineering can be. Two categories of application and fundamental studies are to be discussed.