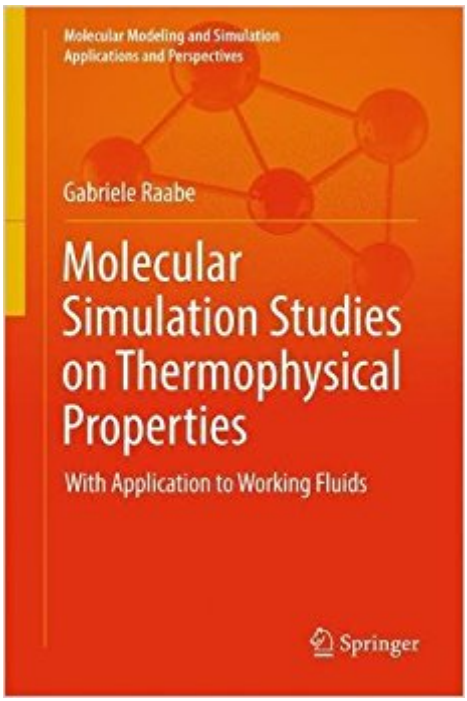
Molecular Simulation Studies On Thermophysical Properties: With Application To Working Fluids (Molecular Modeling And Simulation)



Synopsis

This book discusses the fundamentals of molecular simulation, starting with the basics of statistical mechanics and providing introductions to Monte Carlo and molecular dynamics simulation techniques. It also offers an overview of force-field models for molecular simulations and theirÂ parameterization, with a discussion of specific aspects. The book then summarizes the available know-how for analyzing molecular simulation outputs to derive information on thermophysical and structural properties. Both the force-field modeling and the analysis of simulation outputs are illustrated by various examples. Simulation studies on recently introduced HFO compounds as working fluids for different technical applications demonstrate the value of molecular simulations in providing predictions for poorly understood compounds and gaining a molecular-level understanding of their properties. This book will prove a valuable resource to researchers and students alike.

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Dr. Gabriele Raabe graduated in Mechanical Engineering. She received her Ph.D. in experimental studies on vaporâ “liquid phase equilibria at low temperatures and their modeling by equations of state. She continued to work as thermodynamicist and senior scientist at the Institute for Thermodynamics, TU Braunschweig, and her research activities involve the modeling and prediction of thermophysical properties, focusing on force-field modeling and molecular simulation studies with a wide range of applications that cover, for instance, predicting the thermophysical properties of working fluids and refrigerants, studies on ionic liquids and simulations of drug solubilities. She also has many years of experience in teaching masterâ ™s courses on molecular simulations and thermodynamics of mixtures.

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