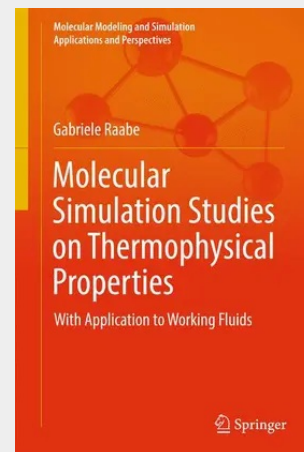


Molecular Simulation Studies on Thermophysical Properties

With Application to Working Fluids

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 their 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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