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Schemes for Coupling Atomic and Continuum Simulations; 9 Fully Analytic Implementation of Density Functional Theory for Efficient Calculations on Large Molecules; 10 Aluminum Nanoparticles: Accurate Potential Energy Functions and Physical Properties; 11 Large-Scale Monte Carlo Simulations for Aggregation, Self-Assembly, and Phase Equilibria
12 New QM/MM Models for Multiscale Simulation of Phosphoryl Transfer Reactions in Solution13 Modeling the Thermal Decomposition of Large Molecules and Nanostructures; 14 Predicting Dynamic Mesoscale Structure of Commercially Relevant Surfactant Solutions; Index

Sommario/riassunto

This book stems from the American Chemical Society symposium, Large Scale Molecular Dynamics, Nanoscale, and Mesoscale Modeling and Simulation: Bridging the Gap, that delved into the latest methodologies and applications for largescale, multiscale, and mesoscale modeling and simulation. It presents real-world applications of simulated and synthesized materials, including organic-, inorganic-, bio-, and nanomaterials, and helps readers determine the best method for their simulation. It gets novices up to speed quickly and helps experienced practitioners discover novel approaches and alte