Multiscale molecular methods in applied chemistry / volume editors, Barbara Kirchner, Jadran Vrabec ; with contributions by R. Abrol

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Abstrak

This book about first-principles-based multiscale, multiparadigm molecular mechanics and dynamics methods for describing complex chemical processes, dynamic QM/MM : a hybrid approach to simulating gas–liquid interactions, multiscale modelling in computational heterogeneous catalysis, real-world predictions from Ab initio molecular dynamics simulations, nanoscale wetting under electric field from molecular simulations, molecular simulations of retention in chromatographic systems : use of biased Monte Carlo techniques to access multiple time and length scales, thermodynamic properties for applications in chemical industry via classical force fields, multiscale approaches and perspectives to modeling aqueous electrolytes and polyelectrolytes, and coarse-grained modeling for macromolecular chemistry.