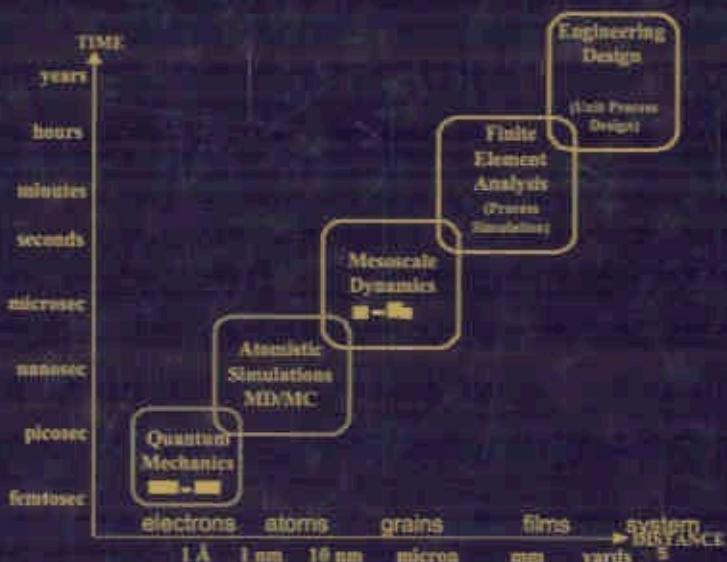


Multiscale Simulation Methods for Nanomaterials



Edited by
RICHARD B. ROSS
SANAT MOHANTY

CONTENTS

Contributors	vii
Preface	xi
1 Overview of Multiscale Simulation Methods for Materials	1
<i>Sanat Mohanty and Richard B. Ross</i>	
2 Influence of Water and Fatty Acid Molecules on Quantum Photoinduced Electron Tunneling in Self-Assembled Photosynthetic Centers of Minimal Protocells	9
<i>A. Tamulis, V. Tamulis, H. Ziock, and S. Rasmussen</i>	
3 Optimizing the Electronic Properties of Carbon Nanotubes Using Amphoteric Doping	29
<i>Bobby G. Sumpfer and Vincent Meunier</i>	
4 Using Order and Nanoconfinement to Tailor Semiconducting Polymers: A Combined Experimental and Multiscale Computational Study	47
<i>Michael L. Drummond, Bobby G. Sumpfer, Michael D. Barnes, William A. Shelton, Jr., and Robert J. Harrison</i>	
5 Coarse Grained-to-Atomistic Mapping Algorithm: A Tool for Multiscale Simulations	73
<i>Steven O. Nielsen, Bernd Ensing, Preston B. Moore, and Michael L. Klein</i>	

6 Microscopic Insights into the Dynamics of Protein–Solvent Mixtures	89
<i>Taner E. Dirama and Gustavo A. Carri</i>	
7 Mesoscale Simulations of Surface-Modified Nanospheres in Solvents	127
<i>Sanat Mohanty</i>	
8 Fixing Interatomic Potentials Using Multiscale Modeling: Ad Hoc Schemes for Coupling Atomic and Continuum Simulations	141
<i>Clifford W. Padgett, J. David Schall, J. Wesley Crill, and Donald W. Brenner</i>	
9 Fully Analytic Implementation of Density Functional Theory for Efficient Calculations on Large Molecules	157
<i>Rajendra R. Zope and Brett I. Dunlap</i>	
10 Aluminum Nanoparticles: Accurate Potential Energy Functions and Physical Properties	169
<i>Nathan E. Schultz, Ahren W. Jasper, Divesh Bhatt, J. Ilja Siepmann, and Donald G. Truhlar</i>	
11 Large-Scale Monte Carlo Simulations for Aggregation, Self-Assembly, and Phase Equilibria	189
<i>Jake L. Rafferty, Ling Zhang, Nikolaj D. Zhuravlev, Kelly E. Anderson, Becky L. Eggimann, Matthew J. McGrath, and J. Ilja Siepmann</i>	
12 New QM/MM Models for Multiscale Simulation of Phosphoryl Transfer Reactions in Solution	201
<i>Kwangho Nam, Jiali Gao, and Darrin M. York</i>	
13 Modeling the Thermal Decomposition of Large Molecules and Nanostructures	219
<i>Marc R. Nyden, Stanislav I. Stoliarov, and Vadim D. Knyazev</i>	
14 Predicting Dynamic Mesoscale Structure of Commercially Relevant Surfactant Solutions	245
<i>Fiona Case</i>	
Index	271