1. Record Nr. UNINA9910140270703321

Titolo	Advances in chemical physics . Volume 155 / / edited by Stuart A Rice, Aaron R Dinner
Pubbl/distr/stampa	Hoboken, New Jersey : , : John Wiley & Sons, , 2014 ©2014
ISBN	1-118-75591-X 1-118-75581-2 1-118-75598-7
Descrizione fisica	1 online resource (298 p.)
Collana	Advances in Chemical Physics ; ; 155
Disciplina	541.394
Soggetti	Chemical kinetics Chemistry, Physical and theoretical Molecular dynamics
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references and indexes.
Nota di contenuto	Advances in Chemical Physics; Contributors to Volume 155; Preface to The Series; Contents; Modeling Viral Capsid Assembly; I. Introduction; A. Virus Anatomies; B. Virus Assembly; 1. Experiments That Characterize Capsid Assembly; 2. Motivation for and Scope of Modeling; II. Thermodynamics of Capsid Assembly; A. Driving Forces; B. Law of Mass Action; 1. Estimating Binding Energies from Experiments; III. Modeling Self-Assembly Dynamics and Kinetics of Empty Capsids; A. Timescales for Capsid Assembly; 1. Scaling Estimates for Assembly Timescales; 2. Lag Times; 3. The Slow Approach to Equilibrium B. Rate Equation Models for Capsid AssemblyC. Particle-Based Simulations of Capsid Assembly Dynamics; D. Conclusions from Assembly Dynamics Models; E. Differences Among Models; F. Higher T Numbers; 1. Structural Stability of Different Capsid Geometries; 2. Dynamics of Forming Icosahedral Geometries; IV. Cargo-Containing Capsids; A. Structures; B. The Thermodynamics of Core-Controlled Assembly; C. Single-Stranded RNA Encapsidation; D. Dynamics of Assembly Around Cores; V. Outlook; References Charges at Aqueous Interfaces: Development of Computational

Approaches in Direct Contact With ExperimentI. Introduction; II. Accounting for Polarizability Effects; A. Models with Explicit Polarization; B. Implicit Polarization via Charge Scaling; C. Beyond Conventional Force Fields; III. Case Studies; A. Hydroxide at Aqueous Interfaces; B. Solvated Electron at the Surface of Water; IV. Outlook; References; Solute Precipitate Nucleation: A Review of Theory and Simulation Advances; I. Introduction; II. Classical Nucleation Theory; A. Homogeneous Nucleation; B. Heterogeneous Nucleation
C. Nucleation TheoremIII. Two-Step Nucleation Theory; A. Metastable Fluid--Fluid Critical Points; B. Phenomenological Theories; C. Coupled Flux Theories and Concentration Fluctuation Gating; IV. Simulation Challenges; A. Landau Free Energies and Rare Events; B. Kramers--Langer--Berezhkovskii--Szabo (KLBS) Theory; C. Nucleus Size in Simulations; D. Which Nucleus Size Metric?; E. Open versus Closed Systems; V. Case Studies; A. Laser-Induced Nucleation; B. Nucleation of Methane Hydrates; C. Nucleation of Calcium Carbonate; VI. Closing Remarks; References
Water in The Liquid State: A Computational ViewpointI. Introduction; II. Potential Energy Functions for Liquid Water; A. Heuristic Models; B. Multisite Models; 1. Three-Site Models; 2. Four-Site Models; 3. Five-Site Models; 4. Six Sites and Beyond; C. Molecular Multipole Models; 1. The Multipole Expansion; 2. The Approximate Multipole Expansion; D. Atomic Multipole Models; E. Summary; III. Multipoles; IV. The Water Molecule in the Pure Liquid; A. Nuclear Geometry; B. Electron Density; C. Multipole Moments; D. Electrostatic Potential; E. Summary; V. Liquid Water; A. Structure; B. Density
C. Thermodynamics

Sommario/riassunto

The Advances in Chemical Physics series provides the chemical physics field with a forum for critical, authoritative evaluations of advances in every area of the discipline. This volume explores the following topics: Modeling Viral Capsid AssemblyCharges at Aqueous Interfaces: Development of Computational Approaches in Direct Contact With ExperimentSolute Precipitate Nucleation: a Review of Theory and Simulation AdvancesWater in the Liquid State: A Computational ViewpointConstruction of Energy Functions for Lattice Heteropolymer Models: Efficient Encodings fo