

1. Record Nr.	UNINA9911009167103321
Autore	Petsev D. N (Dimiter Nikolov), <1962->
Titolo	Molecular theory of electric double layers / / Dimiter N. Petsev, Frank van Swol and Laura J.D. Frink
Pubbl/distr/stampa	Bristol [England] (Temple Circus, Temple Way, Bristol BS1 6HG, UK) : , : IOP Publishing, , [2021]
ISBN	9780750322751 0750322756 9780750322768 0750322764
Edizione	[1st ed.]
Descrizione fisica	1 online resource (various pagings) : illustrations (some color)
Collana	IOP ebooks
Disciplina	541.37
Soggetti	Electric double layer Surface chemistry
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	"Version: 202110"--Title page verso.
Nota di bibliografia	Includes bibliographical references.
Nota di contenuto	1. Introduction : a historical overview -- 1.1. Charges and fields -- 1.2. Electrostatics of systems with distributed charges -- 1.3. The concept of electric double layer part I. Theory. 2. The origin of charge at interfaces involving electrolyte solutions -- 2.1. Effects of the surface chemical reactions and the charge regulation model -- 2.2. Effects due to physical adsorption -- 2.3. Structural effects on the ionic and solvent concentration at the interface 3. Continuum models of the electric double layers -- 3.1. The Poisson-Boltzmann equation -- 3.2. Electric double layer models based on the Poisson-Boltzmann equation : exact and approximate solutions -- 3.3. Beyond the Boltzmann distribution : the semiconductor-electrolyte interface -- 3.4. Electrokinetic phenomena -- 3.5. Deficiencies of the continuum approach 4. Integral equation theory -- 4.1. Background -- 4.2. Percus-Yevick closure -- 4.3. The hypernetted-chain closure -- 4.4. The mean spherical approximation (MSA) -- 4.5. Hard sphere mixtures -- 4.6. The Ornstein-Zernike equations approach to studying electric double layers

5. Perturbation and mean field theory -- 5.1. Background -- 5.2. Virial expansions -- 5.3. Zwanzig's perturbation theory -- 5.4. Mean field theory

6. Density functional theory -- 6.1. Density functional theory for electronic structure -- 6.2. Density functional theory for classical fluids

7. Classical-DFT for electrolyte interfaces -- 7.1. Molecular models of electrolytes -- 7.2. Classical-DFT for point-charge electrolytes -- 7.3. Classical-DFT for finite-size electrolytes -- 7.4. Classical-DFT with correlations -- 7.5. Classical-DFT with cohesive interactions -- 7.6. Classical-DFT for systems with active surfaces -- 7.7. Classical-DFT for water -- 7.8. Classical-DFT for electrokinetic systems

part II. Structure of a single electric double layer : effects due to surface charge regulation and non-Coulombic interactions. 8. Molecular properties of a single electric double layer -- 8.1. Classical density functional theory model of a single flat electric double layer -- 8.2. Solution structure in an electric double layer with surface charge regulation -- 8.3. Conclusions

9. Ionic solvation effects and solvent-solvent interactions -- 9.1. Solvation of the potential determining ions -- 9.2. Solvation of the positive non-potential determining ions -- 9.3. Solvation of the negative non-potential determining ions -- 9.4. Effect of the solvent-solvent fluid interactions -- 9.5. Conclusions

10. Surface solvation and non-Coulombic ion-surface interactions -- 10.1. Solvent-surface interactions. Solvophilic and solvophobic surfaces -- 10.2. Effect of the non-Coulombic interactions between the potential determining ions and the charged wall -- 10.3. Effect of the non-Coulombic positive ions--surface interactions -- 10.4. Effect of the non-Coulombic negative ions--surface interactions -- 10.5. Conclusions

11. The potential distribution in the electric double layer and its relationship to the fluid charge -- 11.1. The Poisson equation for structured electrolyte solutions -- 11.2. Molecular interpretation of the Helmholtz planes, the Stern-Grahame layer, and the electrokinetic shear plane -- 11.3. Conclusions

12. Electric double layers containing multivalent ions -- 12.1. Multivalent ion density profiles in the electric double layer -- 12.2. Effect of the non-potential-determining ions valency on the density profiles of the potential determining ions in the electric double layer -- 12.3. Non-Coulombic surface interactions, charge and potential distributions in the Stern-Grahame layer and beyond -- 12.4. Conclusions

13. Ionic size effects -- 13.1. Ionic size variations and solution density -- 13.2. Conclusions

part III. Numerical methods. 14. Molecular simulation : methods -- 14.1. Background -- 14.2. Molecular dynamics methods -- 14.3. The potential distribution theorem (PDT) -- 14.4. Simulation routes to the grand potential

15. Molecular simulation : applications -- 15.1. Background -- 15.2. One-component plasma -- 15.3. Molten salts -- 15.4. Bulk electrolytes

16. Numerical methods for classical-DFT -- 16.1. Solution methods -- 16.2. Algorithms for constructing phase diagrams.

Sommario/riassunto

The electrical double layer describes charge and potential distributions that form at the interface between electrolyte solutions and the surface of an object, and they play a fundamental role in chemical and electrochemical behaviour. Colloid science, electrochemistry, material science, and biology are a few examples where such interfaces play a crucial role. The focus of this book is on the application of modern liquid state theories to the properties of electric double layers, where it demonstrates the ability of statistical mechanical approaches, such as

the classical density functional theory, to provide insights and details that will enable a better and more quantitative understanding of electric double layers. The book will be essential reading for advanced students and researchers in interfacial science and its numerous applications.
