1. Record Nr. UNINA9911020091803321

Autore	Kaplan I. G (Ilia Grigorevich)
Titolo	Intermolecular interactions : physical picture, computational methods, model potentials / / Ilya G. Kaplan
Pubbl/distr/stampa	Hoboken, NJ, : Wiley, c2006
ISBN	9786610449101 9781280449109 1280449101 9780470300350 0470300353 9780470863343 047086334X 9780470863336 0470863331
Descrizione fisica	1 online resource (381 p.)
Disciplina	541/.394
Soggetti	Molecular dynamics Intermolecular forces
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 index.
Nota di contenuto	Intermolecular Interactions: Physical Picture, Computational Methods and Model Potentials; Contents; Preface; 1 Background Knowledge; 1.1 The Subject and its Specificity; 1.2 A Brief Historical Survey; 1.3 The Concept of Interatomic Potential and Adiabatic Approximation; 1.4 General Classification of Intermolecular Interactions; References; 2 Types of Intermolecular Interactions: Qualitative Picture; 2.1 Direct Electrostatic Interactions; 2.1.1 General expressions; 2.1.2 Multipole moments; 2.1.3 Multipole-multipole interactions; 2.2 Resonance Interaction; 2.3 Polarization Interactions 2.3.1 Induction interactions2.3.2 Dispersion interactions; 2.4 Exchange Interaction; 2.5 Retardation Effects in Long-Range Interactions and the Influence of Temperature; 2.6 Relativistic (Magnetic) Interactions; 2.7 Interaction Between Macroscopic Bodies; References; 3 Calculation of Intermolecular Interactions; 3.1 Large Distances; 3.1.1 Derivation of the

general expression for the multipole expansion of the Coulomb interaction energy operator; 3.1.2 Interaction energy of two atoms in S-states; 3.1.3 Dispersion and induction interactions of molecular systems
3.1.4 Convergence of the multipole expansion3.1.4.1 Perturbation series and the multipole expansion; 3.1.4.2 Study of the convergence of the multipole expansion; 3.1.5 Elimination of divergence in the multipole expansion; 3.2 Intermediate and Short Distances; 3.2.1 Perturbation theory with exchange; 3.2.1.1 Ambiguity of the exchange-perturbation theory series; 3.2.1.2 Symmetry adapted perturbation theories; 3.2.1.3 Methods allowing the standard Rayleigh- Schr odinger perturbation theory to be applied; 3.2.2 Variational methods
3.2.2.1 The Hartree-Fock approximation and accounting for the electron correlation3.2.2.2 Basis set superposition error; 3.2.2.3 Density functional theory; References; 4 Nonadditivity of Intermolecular Interactions; 4.1 Physical Nature of Nonadditivity and the Definition of Many-Body Forces; 4.2 Manifestations of Nonadditive Effects; 4.3 Perturbation Theory and Many-Body Decomposition; 4.3.1 General formulae; 4.3.2 Proof of the additivity of the dispersion energy in the second order of PT; 4.3.3 The dispersion energies of higher orders; 4.4 Many-Body Effects in Atomic Clusters
4.4.1 Rare gas clusters4.4.2 Metal clusters; 4.4.3 Nature of binding in alkaline-earth clusters; 4.4.3.1 Why the study of binding of alkaline-earth elements is important; 4.4.3.2 Nature of binding in dimers and trimers; 4.4.3.3 Population of vacant atomic orbitals; 4.5 Atom-Atom Potential Scheme and Nonadditivity; References; 5 Model Potentials; 5.1 Semiempirical Model Potentials; 5.1.1 Hard-sphere model potentials; 5.1.2 Lennard-Jones potential; 5.1.3 Modifications of the Lennard-Jones potential; 5.1.3.1 (12-6-4) potential; 5.1.3.2 (m-6-8) potential; 5.1.3.3 Kihara potential
5.1.4 Buckingham potential

Sommario/riassunto

The subject of this book - intermolecular interactions - is as important in physics as in chemistry and molecular biology. Intermolecular interactions are responsible for the existence of liquids and solids in nature. They determine the physical and chemical properties of gases, liquids, and crystals, the stability of chemical complexes and biological compounds. In the first two chapters of this book, the detailed qualitative description of different types of intermolecular forces at large, intermediate and short-range distances is presented. For the first time in the monographic literature,