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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,
