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Nota di contenuto	Foundations -- The ideal gas -- Excess function models -- Equation of state models -- Appendix 1 : Fundamental constants and atomic units -- Appendix 2 : Stirling's formula -- Appendix 3 : Relative probability of a microstate -- Appendix 4 : Spherical harmonics, rotation matrices, and clebsch-gordan coefficients -- Appendix 5 : Higher-order perturbation terms for the intermolecular potential energy of simple molecules -- Appendix 6 : Rules for integration -- Appendix 7 : Internal rotation contributions -- Appendix 8 : Quasichemical approximation for the degeneracy in a lattice -- Appendix 9 : Off-lattice formulation of the quasichemical approximation -- Appendix 10 : Combinatorial contribution to the excess entropy in a lattice -- Appendix 11 : Integration variables for three-body interactions -- Appendix 12 : Multipole perturbation terms for the high-temperature expansion.

This book presents the development of modern molecular models for fluids from the interdisciplinary fundamentals of classical and statistical mechanics, of electrodynamics and of quantum mechanics. The concepts and working equations of the various fields are briefly derived and illustrated in the context of understanding the properties of molecular systems. Special emphasis is devoted to the quantum mechanical basis, since this is used throughout in the calculation of the molecular energy of a system. The book is application oriented. It stresses those elements that are essential for practical model development. The fundamentals are then used to derive models for various types of applications. Finally, equation of state models are presented based on quantum chemically based models for the intermolecular potential energy and perturbation theory. The book is suited for graduate courses in chemical and mechanical engineering, physics and chemistry, but may also, by proper selection, be found useful on the undergraduate level.
