1. Record Nr. UNINA9910786225603321 Autore Solana J. R. Titolo Perturbation theories for the thermodynamic properties of fluids and solids / / J.R. Solana Boca Raton, Fla:,: CRC Press, Taylor & Francis Group,, [2013] Pubbl/distr/stampa **ISBN** 0-429-09239-3 1-4398-0776-0 Descrizione fisica 1 online resource (400 p.) Classificazione SCI013050SCI065000 Disciplina 536/.71 Soggetti Thermodynamics Fluids - Thermal properties Solids - Thermal properties Perturbation (Mathematics) Lingua di pubblicazione Inglese **Formato** Materiale a stampa Livello bibliografico Monografia Note generali Description based upon print version of record. Includes bibliographical references. Nota di bibliografia Nota di contenuto Front Cover; Contents; Preface; Author; Notation; Chapter 1: Introduction: Chapter 2: Some Basics on Statistical Mechanics: Chapter 3: Overview of Computer Simulation Methods; Chapter 4: Integral Equation Theories; Chapter 5: Radial Distribution Function and Equation of State of the Hard-Sphere Fluid and Solid; Chapter 6: Free Energy Perturbation Theories for Simple Fluids and Solids; Chapter 7: Perturbation Theories for Simple Fluid Mixtures; Chapter 8: Perturbation Theories for Molecular Fluids; Chapter 9: Inhomogeneous Systems Chapter 10: Overview to Perturbation Theories for More Complex Systems Sommario/riassunto This book, Perturbation Theories for the Thermodynamic Properties of Fluids and Solids, provides a comprehensive review of current perturbation theorie--as well as integral equation theories and density functional theorie--for the equilibrium thermodynamic and structural properties of classical systems. Emphasizing practical applications, the text avoids complex theoretical derivations as much as possible. It begins with discussions of the nature of intermolecular forces and

simple potential models. The book also presents a summary of

statistical mechanics concepts and formulae. In addition, it reviews simulation techniques, providing background for the performance analyses of theories executed throughout the text using simulation data. Chapters describe integral equation theories, theoretical approaches for hard-sphere fluid or solid systems, and perturbation theories for simple fluids and solids for monocomponent and multicomponent systems. They also cover density functional theories for inhomogeneous systems and perturbative and nonperturbative approaches to describe the structure and thermodynamics of hardbody molecular fluids. The final chapter examines several more challenging systems, such as fluids near the critical point, liquid metals, molten salts, colloids, and aqueous protein solutions. This book offers a thorough account of the available equilibrium theories for the thermodynamic and structural properties of fluids and solids, with special focus on perturbation theories, emphasizing their applications. strengths, and weaknesses. Appropriate for experienced researchers as well as postgraduate students, the text presents a wide-ranging yet detailed view and provides a useful guide to the application of the theories described--