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Autore	Elstner Marcus
Titolo	Introduction to Statistical Thermodynamics : A Molecular Perspective / / by Marcus Elstner, Qiang Cui, Maja Gruden
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Nota di contenuto	Part I Microscopic and Macroscopic Theories -- Why Statistical Thermodynamics? -- Energies of Molecules -- Dynamics of molecules -- The laws of thermodynamics -- Principle of maximum entropy -- Part II Fundamentals of Classical Statistical Thermodynamics -- The microscopic entropy -- The Boltzmann distribution -- The canonical distribution -- The canonical ensemble -- Non-interacting and interacting systems -- Part III Application of Classical Statistical Thermodynamics -- State sum (partition function) for non-interacting systems -- Application to ideal gases of polyatomic molecules -- Chemical equilibria and kinetics -- Application to solid bodies -- Application to 2-level systems: spin systems -- Spatial distributions -- Thermodynamics of Real Gases, Liquids and Polymers -- Part IV Quantum statistics and the electronic structure of molecules -- Quantum Statistics -- Electron densities and electron correlations --

	Wave function based methods -- Density Functional Theory (DFT) -- Non-covalent interactions.
Sommario/riassunto	This textbook presents the fundamentals of statistical thermodynamics and electronic structure theory and focuses on introducing the central concepts of thermodynamics and their relation to microscopic theories in a conceptually clear and simple way. The emphasis is on the description of what is going on at the microscopic level, which allows readers to understand the various facets of entropy as the fundamental driving force of all material behaviors. An atomistic perspective is introduced from the beginning, highlighting the importance of molecular structure and microscopic degrees of freedom for understanding the thermodynamic properties of materials, such as heat capacity and magnetization. Because of their importance in various research fields, classical and quantum aspects are treated equally, allowing modern research topics to be addressed with molecular simulation and electronic structure theory. It is a valuable resource for undergraduate and graduate students in chemistry, physics, and materials science, and its modular structure makes it suitable for any reader.