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Autore	Martins, Cidalia
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Nota di contenuto	<p>Collective Electron Dynamics in Metallic and Semiconductor Nanostructures -- Weak Chemical Interaction and van der Waals Forces: A Combined Density Functional and Intermolecular Perturbation Theory #x2013; Application to Graphite and Graphitic Systems -- Reactive Simulations for Biochemical Processes -- Molecular Dynamics Simulations of Liquid-Crystalline Dendritic Architectures -- Surface Diffusion on Inhomogeneous Surfaces -- Electronic, Magnetic and Spectroscopic Properties of Vanadium, Chromium and Manganese Nanostructures -- Electronic Structure and Magnetism of Double Perovskite Systems -- Effect of Spin-Orbit Coupling on the Magnetic Properties of Materials: Theory -- Effect of Spin-Orbit Coupling on the Magnetic Properties of Materials: Results -- Nanostructural Units in Disordered Network-Forming Materials and the Origin of Intermediate Range Order.</p>
Sommario/riassunto	<p>The book covers a variety of applications of modern atomic-scale modeling of materials in the area of nanoscience and nanostructured systems. By highlighting the most recent achievements obtained within a single institute, at the forefront of material science studies, the authors are able to provide a thorough description of properties at the nanoscale. The areas covered are structural determination, electronic excitation behaviors, clusters on surface morphology, spintronics and disordered materials. For each application, the basics of methodology are provided, allowing for a sound presentation of approaches such as density functional theory (of ground and excited states), electronic transport and molecular dynamics in its classical and first-principles forms. The book is a timely collection of theoretical nanoscience contributions fully in line with current experimental advances.</p>