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Titolo	Computational Materials Science [[electronic resource]] : From Basic Principles to Material Properties / / edited by Wofram Hergert, Arthur Ernst, Markus Däne
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Collana	Lecture Notes in Physics, , 0075-8450 ; ; 642
Disciplina	620.1/1011
Soggetti	Condensed matter Materials science Mathematical physics Engineering Condensed Matter Physics Characterization and Evaluation of Materials Theoretical, Mathematical and Computational Physics Engineering, general
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Nota di contenuto	Introduction -- Density Functional Theory and the Full-Potential Local-Orbital Approach -- Methods for Band Structure Calculations in Solids -- A Solid-State Theoretical Approach to the Optical Properties of Photonic Crystals -- Simulation of Active and Nonlinear Photonic Nanomaterials in the Finite-Difference Time-Domain Framework -- Symmetry Properties of Electronic and Photonic Band Structures -- From the Cluster to the Liquid: Ab initio Calculations on Realistic Systems Based on First-Principles Molecular Dynamics -- Magnetism, Structure and Interactions at the Atomic Scale -- Present-Day Achievements of Molecular Dynamics Simulations -- Computational Materials Science with 'Materials Studio': Applications in Catalysis -- Integration of Modelling at Various Length and Time Scales -- Simulation of Material Behaviour from the Engineering Viewpoint - Classical Approaches and New Trends -- Parallel Implementation

	Strategies for Algorithms from Scientific Computing -- Multi-Grid Methods - An Introduction.
Sommario/riassunto	Computational Physics is now a discipline in its own right, comparable with theoretical and experimental physics. Computational Materials Science concentrates on the calculation of materials properties starting from microscopic theories. It has become a powerful tool in industrial research for designing new materials, modifying materials properties and optimizing chemical processes. This book focusses on the application of computational methods in new fields of research, such as nanotechnology, spintronics and photonics, which will provide the foundation for important technological advances in the future. Methods such as electronic structure calculations, molecular dynamics simulations and beyond are presented, the discussion extending from the basics to the latest applications.