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Soggetti	Materials science Mathematical physics Engineering—Materials Chemistry, Physical and theoretical Atoms Physics Solid state physics Characterization and Evaluation of Materials Theoretical, Mathematical and Computational Physics Materials Engineering Theoretical and Computational Chemistry Atomic, Molecular, Optical and Plasma Physics Solid State Physics
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Nota di contenuto	Dedication -- Preface -- Introduction -- Computation of Group Theoretical Properties Using "GAP" -- Some Preliminaries -- Application 1: Identification of Wave Functions to Irreducible Representations -- Application 2: A Systematic Way of the Material Designing -- Technical Details -- Symmetry in C60 -- Analysis of Vibrational Mode in C60 -- Final Remarks -- Appendices A-J.
Sommario/riassunto	This book is intended as an introductory lecture in material physics, in which the modern computational group theory and the electronic

structure calculation are in collaboration. The first part explains how to use computer algebra for applications in solid-state simulation, based on the GAP computer algebra package. Computer algebra enables us to easily obtain various group theoretical properties, such as the representations, character tables, and subgroups. Furthermore it offers a new perspective on material design, which could be executed in a mathematically rigorous and systematic way. The second part then analyzes the relation between the structural symmetry and the electronic structure in C₆₀ (as an example of a system without periodicity). The principal object of the study was to illustrate the hierarchical change in the quantum-physical properties of the molecule, which correlates to the reduction in the symmetry (as it descends down in the ladder of subgroups). The book also presents the computation of the vibrational modes of the C₆₀ by means of the computer algebra. In order to serve the common interests of researchers, the details of the computations (the required initial data and the small programs developed for the purpose) are explained in as much detail as possible. .
