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Soggetti	Perovskite (Mineral) Materials science - Data processing Materials - Analysis Density functionals Mathematical physics Computer simulation Perovskites Computational Materials Science Materials Characterization Technique Density Functional Theory Computational Physics and Simulations
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Nota di contenuto	Calculation methods: Monte Carlo Simulation and Ab Initio Calculations -- Magnetocaloric Effect, Electronic and Magnetic Properties in Manganite Perovskites -- Study of Magnetocaloric Effect, Electronic and Magnetic Properties of Ferrite Perovskites -- Magnetic and Magnetocaloric, Electronic, Magneto-optical, and Thermoelectric Properties of Perovskite Chromites -- Magnetic Properties and Magnetocaloric in Double Perovskite Oxides -- Magnetocaloric and Magnetic Properties of Bilayer Manganite -- Magnetocaloric Properties of Surface Effects in Perovskites Ferromagnetic Thin Films -- Effect of Magnetic Field on the Magnetocaloric and Magnetic Properties of Orthoferrites Perovskite.

Sommario/riassunto

This book undertakes an extensive exploration of manganese-based compounds, such as $TSrxMnO$ ($T = La, Pr$; $x = 0.35, 0.25$) using density functional theory and Monte Carlo simulations with a focus on understanding their electronic, magnetic, and magnetocaloric properties. $BaSrxFeO$ ($x = 0, 0.2$) is also studied via different approximations, offering a comparative perspective. In addition, the book looks at the influence of magnetism using Monte Carlo simulations, revealing crucial parameters and examining the $GdCrO$ system through DFT and Monte Carlo simulation, shedding light on recent experimental observations. Additionally, Monte Carlo studies investigate magnetic and magnetocaloric features of $SrFeMoO$, $LaSrMnO$ bilayer manganite, perovskite ferromagnetic thin films' surface effects, and $SmFeMnxO$ perovskite. In essence, this book significantly advances our comprehension of magnetic and magnetocaloric phenomena across diverse materials and is well-suited for both experimentalists and computational researchers working in this field.
