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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.