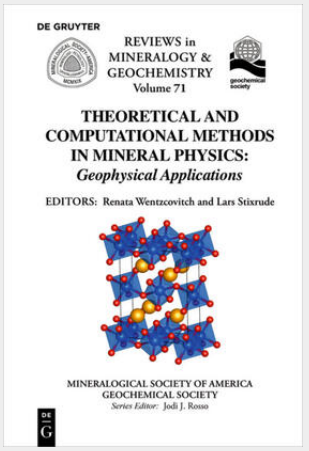
Stixrude / Wentzcovitch

Theoretical and Computational Methods in Mineral Physics

Geophysical Applications



Volume 71 of Reviews in Mineralogy and Geochemistry represents an extensive review of the material presented by the invited speakers at a short course on Theoretical and Computational Methods in Mineral Physics held prior (December 10-12, 2009) to the Annual fall meeting of the American Geophysical Union in San Francisco, California. The meeting was held at the Doubletree Hotel & Executive Meeting Center in Berkeley, California. Contents: Density functional theory of electronic structure: a short course for mineralogists and geophysicists The Minnesota density functionals and their applications to problems in mineralogy and geochemistry Density-functional perturbation theory for quasi-harmonic calculations Thermodynamic properties and phase relations in mantle minerals investigated by first principles quasiharmonic theory First principles quasiharmonic thermoelasticity of mantle minerals An overview of quantum Monte Carlo methods Quantum Monte Carlo studies of transition metal oxides Accurate and efficient calculations on strongly correlated minerals with the LDA+U method: review and perspectives Spin-state crossover of iron in lower-mantle minerals: results of DFT+U investigations Simulating diffusion Modeling dislocations and plasticity of deep earth materials Theoretical methods for calculating the lattice thermal conductivity of minerals Evolutionary crystal structure prediction as a method for the discovery of minerals and materials Multi-Mbar phase transitions in minerals Computer simulations on phase transitions in ice Iron at Earth's core conditions from first principles calculations First-principles molecular dynamics simulations of silicate melts: structural and dynamical properties Lattice dynamics from force-fields as a technique for mineral physics An efficient cluster expansion method for binary solid solutions: application to the halite-silvite, NaCl-KCl, system Large scale simulations Thermodynamics of the Earth's mantle

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