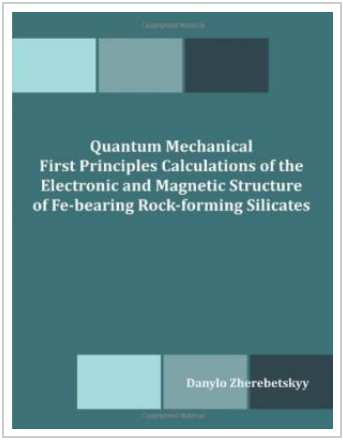

Quantum Mechanical First Principles Calculations of the Electronic and Magnetic Structure of Fe-Bearing Rock-Forming Silicates (Paperback)

By Danylo Zherebetskyy

DISSERTATION.COM, United States, 2010. Paperback. Condition: New. Language: English . Brand New Book ***** Print on Demand *****.The focus of this thesis is the study of the electronic and magnetic structure of three representative members of Fe-bearing rock-forming silicates, viz. orthoferrosilite (Fe2+2Si2O6), almandine (Fe2+3Al2(SiO4)3) and andradite (Ca3Fe3+2(SiO4)3). These minerals have attracted significant attention due to their abundance in the Earth s crust and mantle, and because crystallised silicates are main components of cosmic dust which is the most abundant raw material in the Universe. For this purpose quantum mechanical first principles electronic structure calculations are performed by the most efficient DFT method in the local spin-density approximation for calculating spectroscopic data: the spin-polarized self consistent charge Xa method. The specific feature and strength of these investigations consist in the theoretical characterization of these complex systems based on experimental results. This means that, on one hand, experimental spectroscopic and crystallographic data are being used to judge the reliability of the calculations, whereas, on the other hand, experimental data are interpreted and explained by the theoretical results. This work comprises seven chapters. After a brief introduction (Chapter 1) Chapter 2 describes the theoretical bases, ideas, approximations and advantages of the SCC- Xa...

Reviews

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