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Density functional theory calculations for the electronic, magnetic and chemical bonding properties of geometrically frustrated spinel $CdCr_2O_4$

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Density functional calculations were performed to investigate the effects of magnetic ordering on the electronic structure and bonding properties of $CdCr_2O_4$ with non-magnetic Cd cations and magnetic Cr cations from a pyrochlore lattice. We calculated the electronic structures, magnetic properties and chemical bonding properties of geometrically frustrated Spinel $CdCr_2O_4$ using density functional method combined with the spin-polarized density functional theory, and compared our results in both cubic and tetragonal structures. In order to optimize the crystal structures of spinel $CdCr_2O_4$, we used the plane-wave ultrasoft pseudopotential technique within the generalized gradient approximation (GGA). The exchange and correlation potential was described within the generalized gradient approximation (GGA) based on exchange-correlation energy optimization to calculate the total energy, and the effect of magnetism were obtained and analyzed on the basis of total density of states (DOS), partial density of states (PDOS), and charge density distribution within paramagnetic, ferromagnetic and antiferromagnetic orderings. Also, the electronic charge density distribution in the (1 1 0) crystallographic planes were obtained, for both cubic and tetragonal structures, to explain and compare the bonding properties of spinel $CdCr_2O_4$ in PM, FM, and AFM orderings.

Biography

Najmeh Bolandhemat has completed her MSc in Condensed Matter from Shiraz University, Iran, and is in her last year of PhD in Materials Science in the Department of Physics, Universiti Putra Malaysia (UPM). Prior to moving to Malaysia as a PhD student, she was a Research Assistant in Shiraz University, and Instructor of General Physics, Solid State Physics, Principle of Modern Physics and Electromagnetism laboratory in Fars Science and Research Branch University. Currently, she is a Research Assistant in Science Faculty of UPM University.

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