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A first-principles study on the structural and electronic properties of $CdCr_2O_4$ from density functional theory

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A First-principles Study on the Structural, and Electronic Properties of $CdCr_2O_4$ from Density Functional Theory: In this research, we have investigated the structural, and electronic properties of geometrically frustrated Spinel $CdCr_2O_4$ with cubic ($Fd3m$) and tetragonal ($I4^1/amd$) structures using a pseudopotential plane wave (PP-PW) method within the generalized gradient approximation (GGA). We optimized the crystal structures with the FM and AFM orderings, and computed the electronic properties to investigate the magnetic properties in the geometrically frustrated ferromagnetic and antiferromagnetic spinel $CdCr_2O_4$ using density functional theory and understanding of the principles of Quantum ESPRESSO in magnetic materials. On the other hand, the effect of magnetism were obtained and analyzed on the basis of charge density distribution, density of states (DOS), and project density of states (PDOS).

Biography

Najmeh Bolandhemat has completed her MSc in Condensed Matter from Shiraz University, Iran, and is in her 3rd year of PhD in Materials Science in 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, Principle of Modern Physics, and Electromagnetism laboratory in Fars Science and Research branch University as well as Sarvestan University. Currently, she is a Research Assistant in UPM University with a publication in the *Journal of Computational and Theoretical Nanoscience* (JCTN), and another one in process of being published (accepted) in *PhysicaA; statistical mechanics and its applications*.

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