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Ab-intitio studies of electronic properties of chalcogenide spinels. MAIRBEK CHSHIEV, Y.-H. A. WANG, ARUNAVA GUPTA, Center for Materials for Information Technology, University of Alabama, Tuscaloosa, AL, JOANNA BETTINGER, YURI SUZUKI, Department of Materials Science and Engineering, UC Berkeley, Berkeley, CA, WILLIAM H. BUTLER, Center for Materials for Information Technology, University of Alabama, Tuscaloosa, AL — $CuCr_2Se_4$ is a normal chalcogenide spinel which exhibits ferromagnetic properties including a relatively high Curie temperature of 450 K [1] which makes it a promising candidate for use in spintronics devices. Another chalcogenide spinel of enhanced interest for spintronics is $CdCr_2Se_4$ which seems to be a promising ferromagnetic semiconductor for electrical spin injection into III-V device heterostructures [2]. We report first principles calculations of the electronic structure of substoichiometric $CuCr_2Se_{4-x}$ and $Cu_xCd_{1-x}CrSe_4$ spinels. The calculations were performed using the Vienna ab-initio simulation program (VASP) within the Generalized Gradient Approximation (GGA) of Density Functional Theory (DFT). Our calculations indicate that both Se deficient $CuCr_2Se_{4-x}$ as well as $Cu_xCd_{1-x}CrSe_4$ show half-metallic behavior over a wide range of $x$with a gap around the Fermi level in the minority density of states. [1] F.K. Lotgering, Solid State Commun. 2 (1964) 55 [2] G. Kioseoglou et al., Nature Materials 3 (2004) 799

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