Abstract Submitted
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Ab Initio Study of Magnetic Properties of Cr-doped Chalcopyrites: (BeSn, BeGe, MgGe)N_2[1] J. RUFINUS, Widener University, Chester, PA 19013, J. L. DEWINTER, California Polytechnic State University, San Luis Obispo, CA 93407 — A Density Functional Theory within Generalized Gradient Approximation study of three thermodynamically stable Cr-doped (II-IV)-N_2 chalcopyrites: (BeSn, BeGe, MgGe)N_2 was performed. Since the chalcopyrites are ternary materials, there are possibilities of having ferromagnetic or antiferromagnetic configurations, depending on which metal site was substituted by the dopant. The results show both $BeSnN_2$ and $BeGeN_2$ to be ferromagnetic independent of the substitution sites. On the other hand, $MgGeN_2$ was found to be antiferromagnetic for Cr_{Mg} (Cr substitutes Mg site) and ferromagnetic for Cr_{Ge} (Cr substitutes Ge site.)

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