Ab Initio Study of Magnetic Properties of Cr-doped Chalcopyrites: (BeSn, BeGe, MgGe)N$_2$ 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$_M$g (Cr substitutes Mg site) and ferromagnetic for Cr$_G$e (Cr substitutes Ge site.)

$^1$Work supported by the NSF (Grant number ECS-0609129)