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Ab-Initio Study of Magnetic Properties of M-doped (M = Cr or V) $ZnGeN_2$[1] J. RUFINUS, Science Division, Widener University, Chester, PA 19013 — The current interest in the emerging field of semiconductor spintronics is mostly focused on transition metal-doped binary materials. Recently, however, the explorations of transition metal-doped ternary semiconductors have intensified, due to some experimental confirmations of high Curie temperature in chalcopyrite compounds. In ternary materials, there are possibilities of having ferromagnetic or antiferromagnetic configurations, depending on which metal site was substituted by the dopant. A donor (i.e. releasing electrons) will be produced when a metal atom substitutes a lower valent site, while an acceptor (i.e. releasing holes) will be produced when a metal atom substitutes a higher valent site. Only holes are expected to lead to ferromagnetism. A density functional theory within generalized gradient approximation study was performed on M-doped (M = Cr or V) ternary material $ZnGeN_2$. The objective of this study is to determine whether substitutional transition metal in a group II (Zn) site and in a group IV (Ge) site will be ferromagnetic or antiferromagnetic. Our results show that both Cr- and V-doped $ZnGeN_2$ to be ferromagnetic, independent of the substitution sites. Additionally, formation of half-metallic ferromagnetism is possible in this type of material.

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Jeffrey Rufinus
Widener University

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