

Abstract Submitted
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First principles calculations of magnetic properties of Gd-doped ZnSiN¹ J. RUFINUS, Science Division, Widener University, Chester, PA 19013 — Diluted metal-doped chalcopyrite compounds have recently attracted a great attention due to some experimental confirmations on their ability to achieve high temperature ferromagnetism. Such a material would likely play a role in building future spintronic devices. First principles calculations of the magnetic properties of Gd-doped ZnSiN₂, a semiconductor chalcopyrite, have been performed using the density functional theory within generalized gradient approximation. Our results show, independent of the substitutional sites, the lowest energy structure is ferromagnetic.

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