

Abstract Submitted  
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**Ab-Initio Study of Magnetic Properties of Mn-doped MgSiN<sup>1</sup>**

JEFFREY RUFINUS, Widener University — The current interest in the field of semiconductor spintronics is mostly focused on transition metal-doped binary materials. Recently, however, the explorations of transition metal-doped ternary semiconductors have gained attention, due to experimental confirmations of possible high Curie temperature in chalcopyrite compounds. A density functional theory study was performed on Mn-doped ternary material MgSiN<sub>2</sub>. Our results show Mn-doped MgSiN<sub>2</sub> to be antiferromagnetic for Mn<sub>Mg</sub> (Mn substitutes Mg site) and ferromagnetic for Mn<sub>Si</sub> (Mn substitutes Si site).

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