

Abstract Submitted
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Ab-Initio Study of Magnetic Properties of Mn-doped MgSiN¹

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 MgSiN₂. Our results show Mn-doped MgSiN₂ to be antiferromagnetic for Mn_{Mg} (Mn substitutes Mg site) and ferromagnetic for Mn_{Si} (Mn substitutes Si site).

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