

# First principles calculations of cation-ordering effects on electronic band structure of ZnSnN<sub>2</sub> and ZnGeN<sub>2</sub>

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The Zn(Ge,Sn)N<sub>2</sub> semiconductors are closely related to the (Al,Ga,In)N. Both families have band gaps that span the ultraviolet through the visible range. Attention in the II-IV-N<sub>2</sub> has grown recently, with success in synthesizing ZnSnN<sub>2</sub> reported in 2012 [1] and the recognition of some of their unique optoelectronic properties and the potential that provide for designing novel and useful optoelectronic devices [2, 3]. It is also of great interest that several members of the II-IV-N<sub>2</sub> family are made from earth-abundant and nontoxic elements.

We investigate lattice ordering phenomena for Zn(Ge,Sn)N<sub>2</sub> that are based on the wurtzite lattice, under the constraint that the octet rule be preserved. First-principles calculations of the energies of formation show that the differences in the energies of formation between Pna2<sub>1</sub> and Pmc2<sub>1</sub> crystal structures are 13±3 meV/fu (formula unit) for ZnSnN<sub>2</sub> and an order of magnitude larger for ZnGeN<sub>2</sub>, and that for both materials the Pm31 structure, which contains only octet-rule-violating tetrahedra, has a significantly higher energy of formation and a significantly lower band gap. The octet-rule-preserving model predicts a band gap that for ZnSnN<sub>2</sub> is relatively insensitive to cation-ordering. The violations of the octet rule lead to significant narrowing of the band gap. The observation that ZnGeN<sub>2</sub> orders in the Pna2<sub>1</sub> structure is consistent with the larger difference in the energies of formation of the Pna2<sub>1</sub> and Pmc2<sub>1</sub> structures in this case. The cation-ordering effects presented here has important implications for the optical, electronic and lattice properties of all wurtzite-based heterovalent ternaries.

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