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First principles calculations of cation-ordering effects on electronic band structure of ZnSnN2 and ZnGeN2

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The Zn(Ge,Sn)N_2 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_2 has grown recently, with success in synthesizing $ZnSnN_2$ 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_2 family are made from earth-abandant and nontoxic elements.

We investigate lattice ordering phenomena for Zn(Ge,Sn)N_2 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 $Pna2_1$ and $Pmc2_1$ crystal structures are 13±3 meV/fu (formula unit) for $ZnSnN_2$ and an order of magnitude larger for $ZnGeN_2$, and that for both materials the Pm31 structure, which contains only octet-rule-violating tetrahedra, has a significantly higher energy of formation and a signficantly lower band gap. The octet-rule-preserving model predicts a band gap that for $ZnSnN_2$ is relatively insensitive to cation-ordering. The violations of the octet rule lead to significant narrowing of the band gap. The observation that $ZnGeN_2$ orders in the $Pna2_1$ structure is consistent with the larger difference in the energies of formation of the $Pna2_1$ and $Pmc2_1$ 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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