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Energies of formation and electronic band structure of Zn-IV-N_2 semiconductors ATCHARA PUNYA, WALTER R.L. LAMBRECHT, Case Western Reserve University — The II-IV-N_2 semiconductors are expected to have properties closely related to those of the III-N semiconductors. We focus on Zn-IV-N_2 semiconductors with the group IV-element Si, Ge and Sn. The formation energies of the compounds in this series were calculated by the full-potential linearized muffin-tin orbital method with LDA and GGA. Zero point motion corrections were included. Furthermore, the energies of formation of competing Zn_3N_2, Si_3N_4, Ge_3N_4, Sn_3N_4 compounds were also calculated to determine the allowed ranges of the chemical potentials of the elements where the compounds are stable at zero temperature. For comparison, we also calculated the energy of formation of GaN, which is found to be in good agreement with experimental values. All compounds in the series are found to have a large region of stability. The electronic band structures are calculated using the QSGW method. The band gaps span the region from 1.65 - 5.30 eV, increasing from $ZnSnN_2$ to $ZnSiN_2$, with the bandgap of $ZnGeN_2$ close to that of GaN. While $ZnGeN_2$ and $ZnSnN_2$ are direct band gaps semiconductors, $ZnSiN_2$ is found to have an indirect gap slightly smaller than its lowest direct gap. The states near the valence band maximum at Gamma are symmetry labeled and their splittings analyzed in terms of two crystal field parameters. Spin-orbit coupling is found to have negligible effect on these states.

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