Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Electronic band structures and phonons in Cd-IV-N_2 semiconductors[1] SAI LYU, WALTER LAMBRECHT, Case Western Reserve Univ — Heterovalent ternary semiconductors of formula II-IV-N_2 have recently attracted some interest to complement the group III-N nitride semiconductors. Here we study the Cd-IV-N_2 materials with IV=Si,Ge,Sn. Their electronic band structures are calculated in quasiparticle self-consistent GW approximation and full-potential linearized muffin-tin orbital approach. The lattice parameters are calculated with the local density approximation (LDA) and generalized gradient approximation(GGA). We also computed the effective masses of the valence bands and the conduction bands. The symmetry labels of the bands near the Fermi level were determined. The $CdSiN_2$ and $CdGeN_2$ are found to be indirect band gap semiconductors, while $CdSnN_2$is found to be direct band gap semiconductors.The gaps range from deep ultraviolet to shallow infrared.The phonon frequencies at the Brillouin zone center and Raman spectra are also calculated using density functional perturbation theory. The Born effective charges and dielectric constants are also reported.

[1]NSF DMREF-1533957

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Date submitted: 10 Nov 2016 Electronic form version 1.4