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Structure, Electronic Structure and Phonons of ZnSnN2[1] TULA R. PAUDEL , WALTER R. L. LAMBRECHT, Case Western Reserve University — The structure and electronic structure of $ZnSnN_2$ was calculated using density functional theory in the local density density approximation (LDA) and the linearized muffin-tin orbital method (LMTO). The wurtzite lattice constant is found to be slightly greater then that of GaN. The system is found to have small direct band gap of 0.07eV at Γ in LDA. The phonon frequencies at the Γ were calculated by linear response theory and were labeled according to the symmetry. To the best of our knowledge this compound is studied for the first time both experimentally and theoretically. The stability of the compound will be discussed and the structural electronic and vibrational properties will be compared with other members of the Zn-IV-N_2 (IV=Si,Ge) compounds.

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