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Electronic band structure, crystal structure and phonons of ZnSiN₂¹ TULA R. PAUDEL, WALTER R. L. LAMBRECHT, Case Western Reserve Univ — ZnSiN₂ is an interesting alternative to GaN. Its crystal structure is derived from the wurtzite structure of GaN by a particular ordered substitution of the Ga atoms by Zn and Si in such a way that each N is coordinated with two Si and two Zn atoms. Electronic structure calculations were performed with two different approaches, the plane-wave ultrasoft pseudopotential approach and the full-potential linearized muffin-tin orbital method both using the local density approximation (LDA). The structure was fully optimized. The relaxation consists primarily of the N atom finding its optimum position inside its nearest neighbor tetrahedron by making a shorter Si-N and longer Zn-N bond. An indirect LDA band gap of about 3.4 eV is obtained. Thus a gap larger than for GaN is expected. Calculations of the phonons at the center of the Brillouin zone are in progress using the linear response approach. A comparison with ZnGeN₂, which was studied earlier, [W. R. L. Lambrecht et al. Phys Rev. B 72, 155202 (2005)] will be presented.

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