Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Electronic band structure, crystal structure and phonons of $ZnSiN_2$[1] TULA R. PAUDEL, WALTER R. L. LAMBRECHT, Case Western Reserve Univ — $ZnSiN_2$ is an interesting alternative to GaN. Its crystal structure is derived from the wurtzite structure of GaN by a particular ordered subsitution of the Ga atoms by Zn and Si in such as 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 approaximation (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.

[1]Supported by AFOSR

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Date submitted: 30 Nov 2005 Electronic form version 1.4