

Abstract Submitted
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Phase diagram, structure, and electronic properties of $(\text{Ga}_{1-x}\text{Zn}_x)(\text{N}_{1-x}\text{O}_x)$ solid solution¹ LI LI, PHILIP B. ALLEN, Stony Brook University — We studied $(\text{Ga}_{1-x}\text{Zn}_x)(\text{N}_{1-x}\text{O}_x)$ solid solution by Density Functional Theory (DFT). To conduct thermodynamic simulations, we built a database of structures and constructed a Cluster Expansion(CE). The subsequent Monte Carlo simulation gives a calculated phase diagram with a wide miscibility gap and an ordered $x=0.5$ compound. The disordered phase displays strong short range ordering (SRO) at experimental temperatures. We then used snapshots from MC to investigate structural and electronic properties by DFT on large supercells. Consistent with previous theoretical and experimental findings, lattice parameters appear to deviate from Vegard's law with small upward bowing. Bond lengths depend strongly on local environment, with a variation much larger than the difference of bond length between ZnO and GaN. The downward band gap bowing deviates from parabolic by having more rapid onset of bowing at low and high concentrations. Our results show that SRO influences both the structural and electronic properties.

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