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First Principles Phase Diagram Calculation For $\mathbf{Al_xGa_{1-x}N}$
JEREMY NICKLAS, JOHN WILKINS, Ohio State University — First principles phase diagram calculations were performed for the wurtzite and zincblende structures of the quasibinary system AlN-GaN. The cluster expansion method using the code ATAT was performed without and with excess vibrational contributions to the free energy, F_{vib}. The ab initio calculations were performed with VASP using the PAW pseudopotentials with PBE for the exchange and correlation energies. Preliminary results show miscibility gaps for both structures with a decrease in the consolute points, (X_C,T_C), when including F_{vib}. The wurtzite structure is predicted to be approximately symmetric while the zincblende is predicted to be quite assymetric.

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