Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Atomic and electronic structures of $(GaN)_{1-x}(ZnO)_x$ alloys: the role of short-range order[1] JIAN LIU, PHILIP ALLEN, State Univ of NY- Stony Brook — $(GaN)_{1-x}(ZnO)_x$ solid solution is a promising photocatalyst for efficient water splitting under visible illumination. For theoretical modeling, the special quasirandom structure (SQS) method which assumes random site occupancy is widely used. We have previously shown, with density-functional theory (DFT) total energy calculations, cluster expansion, and Monte Carlo simulations, that short-range order (SRO) is significant due to the non-isovalency. Thus it is desirable to include SRO in the construction of supercells. Inspired by the SQS method, we construct the "special quasi-ordered structure" (SQoS) supercells. Subsequent DFT calculations show that the atomic and electronic structures of SQS and SQoS alloys differ significantly. The SRO and (x,T) dependence of the valence band maximum stem mainly from the anti-bonding hybrids of N2p and Zn3d states. This suggests the possibility of engineering the band gap by tuning SRO. We also explore bond length distribution and bond angle variation over the composition-temperature (x,T) phase space using bond valence method (BVM). The validity of our BVM model is tested by DFT total energy calculations.

[1]Supported by DOE grant No. DE-FG02-08ER46550.

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Date submitted: 14 Nov 2014 Electronic form version 1.4