Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

The Atomic and Electronic Structures of GaN:ZnO Alloys[1]
SHUZHI WANG, Computational Research Division, Lawrence Berkeley National Laboratory, LIN-WANG WANG, Lawrence Berkeley National Laboratory —
GaN:ZnO, a kind of nonisovalent alloys, currently holds the record of the water photo-splitting efficiency under visible light. The mechanism of the large band gap bowing of this alloy, however, is still not clear, due to the lack of knowledge of its detailed atomic structure. We developed a charge flow model based on electron counting rule, which describes the ab initio energies of different alloy atomic configurations of GaN:ZnO with an average error of only 7 meV/atom. This model Hamiltonian was used in Monte Carlo (MC) simulations to study the atomic structures of systems containing thousands of atoms. The equilibrium atomic structures from the MC simulations at different temperatures were then used to calculate their electronic structures. We found that at the experimental synthesis temperature of 1100 K, uniform alloy can be formed, albeit with a strong short range ordering. Consequently, their electronic structure is very different from the completely random alloy. The charge flow model was also applied to many other nonisovalent alloy systems with good accuracy.

[1]This work was supported by U. S. Department of Energy BES/SC

Shuzhi Wang
Computational Research Division, Lawrence Berkeley National Laboratory

Date submitted: 20 Nov 2009 Electronic form version 1.4