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Atomic and electronic structures of GaN:ZnO Alloys[1] SHUZHI WANG, LIN-WANG WANG, Lawrence Berkeley National Laboratory — GaN:ZnO is a new class of alloy which currently holds the record for the efficiency of water photo-splitting. The mechanism of the large band gap bowing of this alloy and its detailed atomic structure, which are essential to understand the remarkable performance, however, are still not clear. We developed a model Hamiltonian describing the ab initio energies of different alloy atomic configurations and used it in Monte Carlo simulations to study the atomic structures of systems containing thousands of atoms. The equilibrium atomic structures from the MC simulations at different temperatures are 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. Based on our calculation, we also predict that higher synthesis temperature can yield even lower energy band gap.

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