

Study of donor defects in zinc oxide using density functional theory (DFT)

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Density Functional Theory (DFT) is widely used for the theoretical study of point defects in semiconductors, allowing for the analysis of the energetic stability and electronic effects of dopants based on the material's atomic and electronic structure. In this work, DFT calculations are employed to study Ga and Al substitutional impurities in bulk ZnO crystals. Zinc oxide possesses a wide bandgap, making it highly promising for applications in optoelectronics and transparent electronics. Although the donor behavior of Ga and Al impurities in ZnO is evident, DFT allows for the assessment of the stability of impurity charge states and their ionization energies. This paper investigates the neutral and +1 charge states of Ga_{Zn} and Al_{Zn} substitutional impurity defects in a 32-atom ZnO crystal, based on total energy and electronic structure calculations. The results confirm that both impurities exhibit donor behavior, while ionized configurations are energetically more favorable and lead to a Fermi level shift characteristic of n-type doping. The obtained results are consistent with the typical errors inherent to DFT reported in literature. To correct these discrepancies, we utilized a semi-empirical approach and quantum perturbation theory, which yielded excellent results for the ionization energies of the impurity defects. Overall, the presented analysis clearly demonstrates the utility of DFT calculations in understanding donor alloying tendencies in ZnO.