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Hybrid density functional study of gallium in ZnO DENIS DEMCHENKO, Virginia Commonwealth University — The properties of interstitial and substitutional gallium impurities as well as their complexes in wurtzite ZnO are modeled using hybrid density functional theory. This approach reproduces experimental band gap and avoids any artificial gap corrections necessary when using LDA/GGA/LDA+U methods. We find that the lattice relaxations at the LDA/GGA level can also introduce large errors to the defect formation energies (up to 1.5 eV). The error is particularly large in cases where shallow occupied defect levels are formed and LDA can produce incorrect charges. The correct defect structure therefore should be obtained by relaxation using hybrid DFT method. We find both interstitial and substitutional Ga forming donor-like defect states, with substitutional Ga being energetically favorable. Acceptor-like Zn vacancy has high formation energy in the isolated state but exhibits strong preference to form defect complexes with both substitutional and interstitial gallium. (Ga_i-V_{Zn}) complex acts as a shallow donor, while ($Ga_{Zn} - V_{Zn}$) is a deep acceptor. The low formation energies of both complexes suggests an appreciable degree of self-compensation.

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