

Abstract Submitted
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Impurity complexes and conductivity of Ga-doped ZnO¹ DENIS DEMCHENKO, Virginia Commonwealth University — Using hybrid functional theory compared with experimental measurements, we investigate the influence of gallium impurities and their complexes on electrical properties of ZnO. In contrast to the behavior of isolated Ga impurities and native defects, the calculated formation energies of Ga complexes are consistent with experimental data. We show that for high levels of Ga doping the acceptor behavior of $(\text{Ga}_{\text{Zn}} - \text{V}_{\text{Zn}})$ and $(\text{Ga}_{\text{Zn}} - \text{O}_i)$ complexes explains the conductivity measurements and compensation levels in ZnO. The computed binding energies of these complexes are in agreement with the binding energies obtained from the measurements of the temperature dependence of carrier mobility. The binding energy dependence on the Fermi level, as well as the computed barrier heights for the formation of complexes are also consistent with the latest experiments on annealing of Ga doped ZnO samples. Our results show that the formation of defect complexes is essential for capturing the physics Ga defects in ZnO.

¹This work used computational facilities of the VCU Center for High Performance Computing.

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