Density functional studies on defects in semiconductors

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Intrinsic defects and impurities play an important role on electrical and optical properties of semiconductors. In order to engineer semiconductor materials with specific properties for desired applications, understanding the role of individual defects is important. Using density functional theoretical calculations, we have attempted to understand the role of individual defects in various environments, which is otherwise difficult by experimental techniques alone. ZnO is a wide band-gap semiconductor, attracting much attention for its many useful applications. Its transparent as well as conducting character is interesting for opto-electronic devices, especially for solar-energy applications.

Among Group-I impurities in ZnO, Li has received particular attention, mainly because, Li is the most common unintentional dopant in hydrothermally grown ZnO. In an effort to understand the defect complexes of Li with intrinsic defects, we considered Li at six different interstitial sites (Li_i), including anti-bonding and bond-center sites and also in substitutional sites such as at Zn-site (Li_{Zn}) and at oxygen site (Li_o) in the ZnO matrix. Stability of Li_{Zn} over Li_i is shown to depend on synthetic condition, viz., Li_{Zn} is found to be more stable than Li_i under O-rich conditions. Hybrid density functional calculations performed on Li_{Zn} indicate that it is a deep acceptor with (0/-) transition taking place at 0.74 eV above valence band maximum.

In addition, we considered the formation of Li-pair complexes and their role on electronic properties of ZnO. Our study suggests that at extreme oxygen-rich synthesis condition, a pair of acceptor type Li_{Zn}-complex is found to be stable over the compensating $Li_i + Li_{Zn}$ pair. The stability of complexes formed between Li impurities and various intrinsic defects is also investigated and their role on electronic properties of ZnO has been analyzed. We have shown that a complex between Li_{Zn} and oxygen vacancy has less formation energy and donor-type character and could compensate the holes generated by Li-doping in ZnO. Charge density and electron-localization function analyses have been used to understand the effect of these defects on the ZnO lattice.

Ref:

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