First-principles study of Li defect complexes in ZnO

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A recent experimental study on proton-implanted Li-doped ZnO microwires has shown room temperature ferromagnetic property. X-ray magnetic circular dichroism (XMCD) spectrum shows peaks at O K-edge, suggesting spin-polarization in O atoms. A comparison of measured XMCD specta and simulated spectra by first-principles method shows that the magnetic signal is mainly due to presence of Zn vacancies (V_{Zn}) in the sample [1]. Similar conclusion has been derived earlier [2]. This gives rise to the hypothesis that Li doping helps in stabilizing V_{Zn}. In order to verify the hypothesis we carry out density functional theory (DFT) investigations on Li-doped ZnO system. The stability of defect complexes is analysed by estimating their formation energies at various partial pressure of oxygen atmosphere (see Ref. 3). In order to overcome the limitations of DFT we use empirical postprocessing treatment [4] and the Heyd-Scuseria-Ernzerhof (HSE) hybrid functional approach [5]. Our results show that Li in ZnO favors an interstitial position both as an isolated defect and as a defect complex. The charge transition level (+2/+) of Li interstitial is found to lie in the band gap at 50 meV above the valence band maximum. This suggests that *p*-type condition could be possible in Li-doped ZnO.

References

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