$ZnAl_2O4$ spinel : electronic structure and formation energy of native defects

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$ZnAl_2O_4$ (Gahnite) is a ceramic which is considered as a possible transparent conducting oxide (TCO) due to its wide band gap and transparency for UV. The key physical properties of TCO material are the band gap, which determines the optical transparency and the band mass, that controlls the mobility of the charge carriers. Defects play an important role in controlling the conductivity of a TCO material along with the dopant - which is the main source of conductivity in an otherwise insulating oxide. We discuss the band gap anomaly observed for this spinel and present the band gap calculated using the state of the art GW approximation[1]. Further, a comprehensive first-principles density functional theory study for point defects in $ZnAl_2O_4$ spinel is also presented using the HSE06 hybrid functional. We have investigated the formation energies of intrinsic defects which include the Zn, Al and O vacancy, and the antisite defects: Zn at Al site (Zn_{Al}) and Al at Zn site (Al_{Zn}). The antisite defect Al_{Zn} has the lowest formation energy and acts as a shallow donor, indicating possible n-type conductivity in $ZnAl_2O_4$ spinel by Al doping[2].

[1] H. Dixit, N. Tandon, S. Cottenier, R. Saniz, D. Lamoen, B. Partoens, V. Van Speybroeck and M. Waroquier, New Journal of Physics, **13**, 063002 (2011).

[2] H. Dixit, N. Tandon, S. Cottenier, R. Saniz, D. Lamoen and B. Partoens, Phys Rev. B, **87**, 174101 (2013)