

Abstract Submitted
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A comprehensive ab initio study of doping in bulk ZnO with group V elements GUIDO PETRETTO, FABIEN BRUNEVAL, CEA Saclay, SRMP — Zinc-oxide, despite being a promising candidate for several electronic applications, up to now has provided several challenges to the scientific community, both from an experimental and theoretical point of view [1]. In fact, a reliable p-type doping still has not been achieved and standard density functional theory (DFT) calculations has often provided unsatisfactory results and failed to help in the search for better configurations to obtain such property. To solve the band gap underestimation problem we have made use of the HSE hybrid functional[2], tuning the admixing parameter to match the experimental band gap. Within this framework, we extensively studied the formation and transition energies of group V elements related defects. These include simple substitutional defects X_{O} , X_{Zn} ($X=\text{N, P, As, Sb}$) and complexes of the form $X_{\text{Zn}}-2V_{\text{Zn}}$ and $X_{\text{Zn}}-V_{\text{Zn}}$. The stability of these complexes is also addressed. We show that it is unlikely to obtain good acceptor states from these elements due to deep transition energies and the presence of donor-like defects. [1]Avrutin, V. et al., Proceedings of the IEEE, 98, 1269 (2010) [2]Heyd, J. et al., Journal of chemical physics 118, 8207 (2003)

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