Effect of noble gas defect on the acceptor formation in ZnO

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Owing to fully occupied orbitals, noble gases have been considered chemically inert species which do not affect materials properties. This consideration follows the basic chemistry of bonding and has been widely confirmed by theoretical works demonstrating that the interaction of a noble gas with surfaces of different compounds is mainly limited to a weak van der Waals interaction. Because of this, experimentalists have been using noble gas implantation as a standard reference in comparison to other implanted samples for the understanding effect of implantation-produced structural disorder on a wide range of different materials properties. However, the insertion of a chemically inert species can also result in changing charge density redistribution and eventually affecting material properties[1]. Using first-principles calculations, we investigate the effect of this charge distribution on the relative defect formation energies of different acceptors e.g., ZnO:Ag_{Zn}, ZnO:N_o, ZnO:Li_{Zn}, and ZnO:Na_{Zn}. We demonstrate that in contrast to common beliefs, the presence of noble gas defects in a doped system can reduce the defect formation energies of acceptor defects. This effect originated from (i) the effect of the noble gas defect on localized defect states in ZnO (e.g., delocalization of O vacancy [1]) and (ii) energy lowering due to decay of delocalized electron to the acceptor states. These results demonstrate that noble gas defects cannot be excluded in the analysis of defect stability and compensation mechanism.

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References

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