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Native Point Defects in ZnO

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Abstract : Using first-principles methods based on density functional theory and pseudopotentials, we have performed a details study of native defects in ZnO. Native point defects are unlikely to be cause of the unintentional n-type conductivity. Oxygen vacancies, which considered most often been invoked as shallow donors, have high formation energies in n-type ZnO, in edition are a deep donors. Zinc interstitials are shallow donors, with high formation energies in n-type ZnO, and thus unlikely to be responsible on their own for unintentional n-type conductivity under equilibrium conditions, as well as Zn antisites which have higher formation energies than zinc interstitials. Zinc vacancies are deep acceptors with low formation energies for n-type and in which case they will not play role in p-type coductivity of ZnO. Oxygen interstitials are stable in the form of electrically inactive split interstitials as well as deep acceptors at the octahedral interstitial site under n-type conditions. Our results may provide a guide to experimental studies of point defects in ZnO.

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