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Probing deactivations in Nitrogen doped ZnO by vibrational signatures: A first principles study

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Abstract

Based on first principles calculations, we investigate two probable types of deactivation mechanisms that hinder current efforts of doping ZnO p-type. (i) Passivation by Hydrogen. H prefers to bind with N_O at the anti-bonding site and form N_O–H complexes with a binding energy of about 1 eV. (ii) Passivation by the formation of substitutional diatomic molecules (SDM). Carbon impurities and excess N strongly prefer to passivate N_O and form low-energy SDM on the Oxygen site, $(NC)_O$ or $(N_2)_O$, both of which are donors with several-eV binding energies. Our calculated vibrational frequencies of N_O–H complexes and SDMs are consistent with the frequencies recently observed by IR measurement on N-doped ZnO, which is not p-type.

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