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First-Principles Density Functional Study of Nitrogen-Doped P-Type ZnO

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Abstract : We present a theoretical investigation on the structural, electronic properties and vibrational mode of nitrogen impurities in ZnO. The atomic structures, formation and transition energies and vibrational modes of (NO3)i interstitial or NO4 substituting on an oxygen site ZnO were computed using ab initio total energy methods. Based on Local density functional theory, our calculations are in agreement with one interpretation of bound-excition photoluminescence for N-doped ZnO. First-principles calculations show that (NO3)i defects interstitial or NO4 substituting on an Oxygen site in ZnO are important suitable impurity for p-type doping in ZnO. However, many experimental efforts have not resulted in reproducible p-type material with N2 and N2O doping. by means of first-principle pseudo-potential calculation we find that the use of NO or NO2 with O gas might help the experimental research to resolve the challenge of achieving p-type ZnO.

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