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Mechanism for acceptor compensation and efficient p-type doping in ZnO

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While ZnO exhibits intrinsic n-type conductivity, it is difficult to obtain low resistivity p-type samples. Among group-V elements, N is considered to be a good p-type dopant. Very recently, it has been demonstrated that ZnO can be p-type with P and As impurities. For group-I elements such as Li and Na, substitutional acceptors are known to be compensated by interstitial donors.

In this work, we study the defect properties of both group-I (Li and Na) and group-V (N and P) dopants in ZnO through first-principles pseudopotential calculations within the local-density-functional approximation. Based on the formation energies for various defects, we discuss their stability and defect concentrations as a function of the Fermi level. We examine the hydrogenation and annealing effects on doping efficiency, and provide efficient doping techniques to achieve low-resistivity p-type samples.