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Theoretical study of preferred dopants for n-type transparent conducting oxides SU-HUAI WEI, National Renwable Energy Laboratory, USA, CHONG LI, JINGBO LI, Institute of Semiconductor Physics, CAS, China, WAN-JIAN YIN, YANFA YAN, Department of Physics, University of Toledo, USA —
Traditionally, it is believed that the conduction band edges of d^0 or d^{10} oxides are derived mostly from cation states, thus substitutional doping on anion sites is expected to cause less perturbation and produce shallow donor levels in these materials. Using first-principles calculations, we show that although this paradigm is applicable for more covalent oxides such as SnO_2 where F_O is a better n-type dopant than Sb_{Sn}, for more ionic oxides such as ZnO, the conduction band edge actually contains a considerable amount of O s orbitals, thus F_O in ZnO causes larger perturbation and consequently produces deeper donor levels than cation site doping such as Al_{Zn}. This observation can be explained by coupling of cation state with high lying oxygen orbitals. The origin of the preferred n-type dopability of oxides, the potential of oxygen vacancy as n-type dopant, and the selection of chemical potential for n-type doping will also be discussed.

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