Theoretical study of preferred dopants for n-type transparent conducting oxides

SU-HUAI WEI, National Renewable Energy Laboratory, USA, CHONG LI, JINGBO LI, Institute of Semiconductor Physics, CAS, China, WANJIAN 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.