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Natural off-stoichiometry and asymmetry in p/n-dopability of wide-gap oxides[1] S. LANY, J. OSORIO-GUILLEN, H. RAEBIGER, A. ZUNGER, National Renewable Energy Lab. — Oxides such as In_2O_3 and ZnO can be doped n-type and are naturally anion deficient, while oxides such as NiO and Cu_2O are$p$-type and tend to be naturally metal-deficient. Furthermore, they exhibit the property of transparent conductivity, unlike most oxides. To decipher these phenomena, we perform thermodynamic simulations based on first-principles calculated formation energies of many neutral and charged defects. We find that the metal-vacancies (and not O-interstitials) in NiO and Cu_2O are responsible for their simultaneous metal deficiency and p-type conductivity. The O-deficiency of In_2O_3 and ZnO is caused by the O-vacancy V_O (and not the metal interstitials). Since V_O has a *deep* level in the gap, it does not provide for equilibrium stable n-type conductivity. We suggest, however, that a metastable state of V_O in In_2O_3 and ZnO can cause persistent photoconductivity, and can explain the paradoxical coexistence of coloration (deep absorption level in the optical range) and conductivity (shallow level), which is observed after metal rich growth. By calculating the band offsets, we further show that the p-type dopability of NiO is facilitated by the relative high energy of the valence band maximum, while the n-type dopability of ZnO is facilitated by the relative low energy of the conduction band minimum.

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