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3d impurities in wide gap oxides—magnetism and carrier doping.[1]
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3d transition metal impurities in wide-gap oxides exist in multiple charged configurations[1], and may function as (i) donor/acceptor defects to modify carrier concentrations, (ii) magnetic elements to induce collective magnetism, and (iii) shift the host band edges. While previous investigations have addressed some of these phenomenologies separately, we link them together, and present the chemical trends for electronic properties, carrier doping, and magnetism along the series of 3d1...3d8 impurities in the paradigmatic wide-gap oxide hosts ZnO and In2O3. For these general trends we find that, in In2O3 most 3d impurities are amphoteric and exhibit deep transitions, whereas in ZnO the early 3d impurities (Sc-V) have shallow donor transitions, and only the late 3d's (Co, Ni, Cu) have acceptor transitions inside the band gap. Ferromagnetic interactions emerge upon the partial filling of 3d levels resonant inside the conduction band, an in general require electron doping from additional sources. [1] H. Raebiger, S. Lany, and A. Zunger, Nature **453**, 763 (2008).

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