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Charge regulation via a negative feedback: transition metal atoms in semiconductors and insulators[1] HANNES RAEBIGER, STEPHAN LANY, ALEX ZUNGER, NREL, Golden, CO 80401 — Transition metal (TM) atoms in semiconductors and insulators produce energy levels in the band gap, whose occupation can be altered by shifting the Fermi level e.g. via doping. Changes in level occupation correspond to changes in the formal oxidation state. Such changes are associated with inward/outward lattice relaxations recorded as "ionic radii", different magnetic moments, and a core shift in x-ray photoemission. We show, via density-functional calculations within the plane-wave supercell method for TM atoms including Cr, Mn, Fe, and Co in the semiconductor hosts GaAs and Cu_2O, as well as in the ionic insulator host MgO, that changes in gap-level occupation result in only very small changes of charge on the TM atom itself. We show that this is due to an inherent negative feedback that regulates the TM charge via a TM–ligand rehybridization. Further, the inward/outward lattice relaxations and XPS core shifts, often associated with a change of the TM charge, in fact follow from the TM-ligand rehybridization, as the TM charge is kept unchanged via the inherent negative feedback.

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