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Asymmetric hole localization and multiple hole binding of acceptors in ZnO[1] STEPHAN LANY, ALEX ZUNGER, National Renewable Energy Laboratory — Holes bound at cation-site acceptors in oxides, such as Li_{Zn} or the Zn vacancy in ZnO tend to be localized on a single oxygen neighbor rather than to be delocalized over symmetrically equivalent sites. As a consequence of this localization, the acceptor level lies deep in the gap, typically $\sim$1 eV above the VBM. In contrast, conventional local density calculations do not show this symmetry breaking, and predict the acceptor level much too shallow. This failure of approximate functionals has been attributed to the residual self-interaction, which underestimates the energy splitting between occupied and unoccupied states. We identify a criterion for the cancellation of the self-interaction in terms of a generalized Koopmans theorem, and use this criterion to define a self-interaction correction (SIC) potential that does not rely on empirical parameters. After the SIC, the unoccupied hole states are correctly placed in energy with respect to the spectrum of the occupied host states. We use this method to predict the acceptor levels of cation-site acceptors and the Zn vacancy in ZnO, and of acceptors in In_2O_3 and SnO_2. We find that these acceptors have too deep levels to cause p-type conductivity, and we further predict that nominal single acceptors can generally bind multiple holes (up to 3).

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