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Hybrid functional studies of defects and hole polarons in oxides.

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Transparent conducting oxides (TCOs) are ubiquitous, appearing in windows, flat-panel displays, solar cells, solid-state lighting, and transistors that all exploit TCOs' combination of high electrical conductivity and optical transparency. Thanks to this large and growing list of applications, there has been a surge of interest in the science of these materials, focusing on the fundamental properties and doping opportunities in traditional TCOs as well as the exploration of promising new candidate materials. Hybrid density functional theory has proven instrumental in elucidating the physics of TCOs. One example is the study of dopants and defects that determine the conductivity. Accurate formation energies and charge-state transition levels can now be obtained thanks to the accurate electronic structure provided by a hybrid functional. This allows us to address the origins of unintentional conductivity: for SnO_2, In_2O_3, and Ga_2O_3, we demonstrate that this is *not* due to native defects such as oxygen vacancies, but must be attributed to unintentional incorporation of impurities. We can also provide guidelines for achieving higher doping levels, suggesting several impurities as candidate donors with high solubility. Limitations on doping due to the formation or incorporation of compensating centers are addressed as well. Hybrid functional calculations also overcome the shortcomings associated with traditional local or semi-local functionals, which do not properly describe charge localization. Hybrid functionals accurately describe polaron formation, i.e., the self-trapping of holes when $p-$type doping of the oxide materials is attempted. Consequences of polaron formation for optical characterization of the material will be discussed. This work was performed in collaboration with Anderson Janotti and Chris G. Van de Walle, and was in part under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.