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Doping Rules in A_2BO_4 Spinel Oxides ALEX ZUNGER, T. PAUDEL, V. STEVANOVIC, S. LANY, Natl. Renewable Energy Lab., CO — Many of the physical phenomena surrounding Complex Oxide involve the creation and annihilation of charge carriers by cross –substitution of atoms or by the formation of vacancies and interstitials. We have used the machinery of First-Principles defect calculation, developed and tested over the years on semiconductors (where experimental data needed to test DFT corrections is rather clear), applying it to a large number of oxides, initially from the Spinel family. We calculate defect formation energies as a function of temperature and oxygen partial pressure, as well as the concentration of donors and acceptors and the ensuing free carriers. A number of regularities emerge. (i) Oxygen vacancies are not a viable source of electrons and cation vacancies are (usually) not a viable source of holes. (ii) Instead, cation-antisites (A-on-B donor and B-on-A acceptors) tend to form in significant numbers and release carriers. (iii) For the group of A3+ and B2+ spinels we find four "doping classes" (a) both donor and acceptor are in the gap (Al_2MgO_4) (b) Only acceptor is in the gap (Co_2ZnO_4) (c) only donor in the gap and (d) none in the gap. Simple regularities can be used as first-order rules to guess electrical behavior from composition. This work was supported through the Center for Inverse Design, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences.

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