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The trends of oxygen vacancy levels in metal oxides WANJIAN YIN, SUHUAI WEI, MOWAFAK AL-JASSIM, National Renewable Energy Laboratory, YANFA YAN, Department of Physics, Unviversity of Toledo, OH — Most of the d or d^{10} oxides such as ZnO, SnO_2 , In_2O_3 , and TiO_2 are wide-bandgap *n*-type semiconductors even though they are not intentionally doped. For quite a long time, it was commonly believed that oxygen vacancies (V_O) in metal oxides are the electron donors because the formation energy of V_O in metal oxides is low and the electrical conductivity of the *n*-type oxides is closely linked to the formation of V_O However, recent theoretical and experimental studies have put this point of view in question especially with different calculation methods involved. We present a detailed analysis of the wavefunction characters of oxygen vacancy in conventional metal oxides and unveil the chemical trend of oxygen vacancy transition energy levels with respect to the conduction-band minimum (CBM). We show that in the type-s and type-p metal oxides, where the character of an oxygen vacancy level is similar to that of the CBM, the oxygen vacancy levels are generally deep and become deeper when the cation size decreases. In type-d metal oxides, the oxygen vacancy levels are generally shallow and can sometimes even be above the CBM. Our analysis is confirmed by the calculated trends of oxygen vacancy levels in representative metal oxides using hybrid density functional analysis. It also provides guidelines to search a metal oxide that has shallow V_O donor levels, such as the one found in $BiVO_4$



Prefer Oral Session Prefer Poster Session Wanjian Yin yinwanjian@gmail.com National Renewable Energy Laboratory

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