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First-principles study of native defects in $ZnRh_2O_4$ spinel

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Transparent conducting oxides (TCOs) are widely used for many applications. Typically, most of TCOs are intrinsically n-type semiconductors and are difficult to be doped for p-type conductivity. The spinel $ZnRh_2O_4$ has been recognized as a potential p-type TCO. In this work, we present energetics and electronic properties of native defects including vacancy, interstitial and antisite defects in $ZnRh_2O_4$ by mean of first-principles calculations. Computed pinned Fermi levels are closed to the valence band edge in any possible growth conditions. It is thus difficult to grow an n-type $ZnRh_2O_4$, which is consistent with experimental facts. Based on our calculated formation energies, we observe that the Zn vacancy (V_{Zn}) acts as a deep acceptor and has relatively high formation energy, and thus V_{Zn} is unlikely to be responsible for the p-type conductivity. By contrast, we find that Zn substituting for Rh (Zn_{Rh}) acts as an acceptor forming a shallower transition level than that of V_{Zn}. Under O-rich/Rh-poor and Zn-rich/O-poor conditions, Zn_{Rh} is found to be the major source of unintentional p-type conductivity in $ZnRh_2O_4$. To enhance hole concentration, we suggest experimentalists to grow $ZnRh_2O_4$ under high oxygen partial pressure with low Rh concentration.

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