

Abstract Submitted  
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**Self-trapping of holes in p-type oxides: Theory for small polarons in MnO**<sup>1</sup> HAOWEI PENG, STEPHAN LANY, National Renewable Energy Laboratory — Employing the  $p$ - $d$  repulsion to increase the valence band dispersion and the energy of the VBM is an important design principle for p-type oxides, as manifested in prototypical  $p$ -type oxides like  $\text{Cu}_2\text{O}$  or  $\text{CuAlO}_2$  which show a strong  $\text{Cu-}d/\text{O-}p$  interaction. An alternative opportunity to realize this design principle occurs for  $\text{Mn}(+\text{II})$  compounds, where the  $p$ - $d$  orbital interaction occurs dominantly in the fully occupied  $d^5$  majority spin direction of Mn. However, the ability of Mn to change the oxidation state from +II to +III can lead to a small polaron mechanism for hole transport which hinders p-type conductivity. This work addresses the trends of hole self-trapping for MnO between octahedral (rock-salt structure) and tetrahedral coordination (zinc-blende structure). We employ an on-site hole-state potential so to satisfy the generalized Koopmans condition. This approach avoids the well-known difficulty of density-functional calculations to describe correctly the localization of polaronic states, and allows to quantitatively predict the self-trapping energies. We find that the tetrahedrally coordinated Mn is less susceptible to hole self-trapping than the octahedrally coordinated Mn.

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