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Multivalency of group-V elements in SnO_2[1] HAOWEI PENG, STEPHAN LANY, National Renewable Energy Laboratory — Multivalence is an intrinsic property of elements being capable to change their valence state which usually companies with environmental perturbation such as lattice distortion. It commonly shows in transition metal compounds, but also in some some main-group elements, especially heavy group-IV and -V elements. Group-V elements were proposed as n-type dopants in SnO_2, and compared with the commercial FTO (F-doped SnO_2), the cation-site incorporation can facilitate various growth techniques. However, substituting for Sn^{4+} ions, the group-V elements can possess either the desired 5+ oxidation state that generates electron charge carriers, or a compensating 3+ oxidation state. Hence, specific attention to this multivalence characteristics is indispensable. To this end, we accurately determine the defect transition energy level $\epsilon(1-/1+)$ with respect to the conduction band minimum, by combining the state-of-art quasiparticle GW and hybrid functional calculations. Group-V elements including P, As, Sb and Bi are considered, which have strong site-preference on Sn instead of on O sites.

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