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The nature of Group-V acceptor impurities in SnO_2[1] JOEL VARLEY, Department of Physics, University of California at Santa Barbara, ANDERSON JANOTTI, CHRIS VAN DE WALLE, Materials Department, University of California at Santa Barbara — Group-V elements have long been considered leading candidates for achieving p-type doping in semiconducting oxides. Using first-principles calculations, we investigate the feasibility of achieving ambipolar doping in SnO_2 using the Group-V elements N, P, and As. We address the electronic structure of these impurities by performing systematic density functional calculations using hybrid functionals. This approach overcomes the band-gap problems inherent in calculations using the local density approximation or generalized gradient approximation, thus allowing us to accurately determine energies of defect levels. We discuss the stability of the isolated impurities both as substitutional and interstitial defects, based on calculated formation and migration energies. We also investigate their possible passivation by hydrogen and examine binding energies and activation energies of hydrogen-acceptor complexes. We conclude that the Group-V elements are deep acceptors that will not enable p-type doping of SnO_2.

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