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Group III-A Acceptor-Hydrogen interactions in SnO_2 JOEL VARLEY, Physics Department, University of California, Santa Barbara, CA 93106, ANDERSON JANOTTI, ABHISHEK SINGH, CHRIS G. VAN DE WALLE, Materials Department, University of California, Santa Barbara, CA 93106 — Using first-principles calculations we investigate the role of hydrogen in the passivation of p-type dopants in SnO_2. We focus on group III-A elements, including Al, Ga, and In and investigate the stability of these impurities when substituting Sn under hydrogen-free and hydrogen-rich conditions. Hydrogen effectively passivates the acceptors and removes their electrical activity. Based on calculated binding and migration energies we discuss conditions under which hydrogen can be removed and acceptor activation can take place. We also calculate the stretch-mode vibrational frequencies associated with the hydrogen-impurity complexes, providing a signature for experimental identification in vibrational spectroscopy. We conclude that the group III-A elements studied are suitably shallow acceptors for p-type doping and that the presence of interstitial H will not impede, and potentially enhance, p-type doping of SnO_2.

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