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O-Vacancy-H_2 Complex in ZnO as the Electrically Inactive Hidden Hydrogen Species and its Activation

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I investigate the defect complexes in ZnO, consisting of an oxygen-vacancy and a hydrogen pair, using the density-functional theory calculations. In H-rich *n*-type ZnO, the oxygen-vacancy-dihydrogen (V_O-H_2) complex in the configuration of the two Zn-H-Zn bonds is found to be more stable than the H substitutional at the oxygen site (H_O^{1+}) or the H interstitial (H_i^{1+}) in its lowest energy configuration. The V_O-H_2 complex is a deep double donor and electrically inactive in the ground state. However, upon excitation, the ionized $(V_O\text{-}H_2)^{2+}$ is found to decompose into the two atomic forms of H_O^{1+} and H_i^{1+}. The experimentally observed photo-sensitivity of the g=1.96 shallow donor electron-spin-resonance and the observed increase of the atomic H interstitials during the thermal annealing of hydrogenated ZnO can be explained with the V_O-H_2 model.