Abstract Submitted
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Hydrogen dynamics in indium oxide[1] W.B. FOWLER, M. STAVOLA, WEIKAI YIN, Lehigh University — It has been recognized that hydrogen is a shallow donor in several transparent oxides, including In_2O_3 [1]. Both interstitial H and H at an O vacancy have been suggested as candidates [2]. We have used the CRYSTAL06 code[3] with a hybridized DFT Hamiltonian to determine equilibrium positions and vibrational frequencies for both of these cases as well as for H at an In vacancy. While the bixbyite structure [4] of In_2O_3 has overall cubic symmetry, its remarkable internal asymmetries lead to a number of candidate locations for the H, each of which has different vibrational frequencies. This enables potential assignments of the experimental IR results obtained by Yin *et al* [5]. Furthermore, the unique topology of In_2O_3 leads to constraints on possible H diffusion paths, which we have also investigated.

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