Hydrogen dynamics in indium oxide

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$_2$O$_3$ [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$_2$O$_3$ 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$_2$O$_3$ leads to constraints on possible H diffusion paths, which we have also investigated.


$^1$Supported by NSF grant DMR-1160756.