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Dynamics of H_i^+ in Indium Oxide[1] W. B. FOWLER, M. STAVOLA, YING QIN, P. WEISER, WEIKAI YIN, Lehigh University — Studies of IR absorption[1] under uniaxial stress[2] and diffusion[3] of H_i^+ as well as the dynamics of positively charged muonium[4] in In_2O_3 provide an experimental framework to understand these processes in detail. While the bixbyite structure[5] of In_2O_3 has overall cubic symmetry, its remarkable internal asymmetries lead to a number of candidate locations for H_i^+. Furthermore, the unique topology of In_2O_3 leads to constraints on possible H diffusion paths. We have used the CRYSTAL06 code[6] with a hybridized DFT Hamiltonian to determine equilibrium positions and vibrational frequencies for possible sites for H_i^+ and have analyzed candidate diffusion paths and processes for H_i^+ and Mu^+.[1] W. Yin *et al.*, Phys. Rev. B **91**, 075208 (2015). [2] P Weiser *et al.*, this meeting. [3] Ying Qin *et al.*, this meeting. [4] B. B. Baker *et al.*, AIP Conf. Proc. **1583**, 323 (2014). [5] M. Marezio, Acta Crystallogr. **20**, 723 (1966). [6] R. Dovesi *et al.*, *Crystal06 User's Manual* (University of Torino, Torino, 2006).

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