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Vibrational properties of an OH center in β $-\mathbf{Ga_2O_3}$[1] W. B. FOWLER, P. WEISER, M. STAVOLA, Lehigh University — Theoretical predictions suggest that hydrogen impurities play a crucial role in the electrical conductivity of $\beta-Ga_2O_3$ by acting as shallow donors and by passivating cation-vacancy acceptor complexes [1,2]. IR spectroscopy of $\beta-Ga_2O_3$ single crystals treated in an H_2 (D_2) ambient display a strong vibrational line at 3437 (2546) cm^{-1} originating from an O-H(D) containing defect. This line is thermally stable at 1000C, which suggests that it may arise from a V_{Ga}-H complex. Theoretical calculations using the CRYSTAL06 code [3] with hybridized DFT Hamiltonian and the polarization properties of the O-H vibrational line are used to determine possible microscopic structures for this defect and other possible defects. [1] J. B. Varley *et al.*, Appl. Phys. Lett. **97**, 142016 (2010). [2] J. B. Varley *et al.*, J. Phys.: Condens. Matter **23** (2011), 334212. [3] R. Dovesi *et al.*, *Crystal06 User's Manual* (University of Torino, Torino, 2006).

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