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**Dynamics of Interstitial H in $TiO_2$**[1] W.B. FOWLER, A. MURPHY[2], M. STAVOLA, Lehigh Univ. — H transport in rutile $TiO_2$ is important because of the low energy barriers within the open lattice in the c-direction [1]. As part of a study of the dynamics of interstitial H, potential energy functions for the vibration of hydrogen between two cross-channel O were generated. Double-well functions were modeled using experimental data [2] for the fundamental stretching vibrational frequencies of the three isotopes of H along with theoretical information obtained from quantum-mechanical calculations using [3] CRYSTAL06. These functions were then used to predict where the first overtone may lie, and its relative transition probability. The unexpectedly large anharmonicity observed for the OH vibration is correlated with the hydrogen-bond nature of the O-H —-O potential.

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