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Hydrogen-related defects in SnO_2[1] W. BEALL FOWLER, FIGEN BEKISLI, MICHAEL STAVOLA, Lehigh University — Symmetry arguments along with a mass-and spring analysis of infrared absorption experiments made with polarized light on OH defects in SnO_2 yield significant insights into the possible structures of one- and two-OH defects that have been observed recently [1]. Namely, a two-OH defect must involve symmetry-equivalent OH sites, and the axes of both one- and two-OH defects are only slightly displaced from the perpendicular to the c-axis of the rutile structure. Such results cannot be explained by models involving one or two H trapped at a Sn vacancy. Rather, they are consistent with OH defects associated with either a metal atom substituting for Sn, or an interstitial metal atom (such as Sn). Results of detailed quantum-mechanical calculations [2] using CRYSTAL06 are consistent with OH structures involving a Sn interstitial.

[1] Figen Bekisli *et al.,* Phys. Rev. B **84**, 035213 (2011).
[2] R. Dovesi *et al.*, ***Crystal06 User's Manual***, Univ. of Torino, Torino, 2006.

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