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Unambiguous identification of an OH-Li center in ZnO: Theory[1]
W.B. FOWLER, G.A. SHI, M. STAVOLA, Lehigh University — Three structures[1] have been suggested for the OH-Li complex in ZnO whose Li isotope shift has been observed by Shi, Stavola, and Fowler: (a), an O-H-second neighbor Li; (b), Li-O-H; and (c), O-H-Li (a bond-centered hydrogen), with all three atoms along the c-axis. Wardle *et al.* [2] have theoretically investigated the energies of two of these structures. They found (c) to be the ground state and (b) to be 0.5 eV higher in energy. We have used[3] CRYSTAL2003 to evaluate the structural and vibrational properties of this defect. We also find the ground state to be bond centered, with structure (b) higher in energy by 0.5 eV and structure (a) higher by 0.7 eV. We have then moved the O, H, and Li atoms by hand along the c-axis to obtain harmonic force constants and anharmonic constants and have used the harmonic force constants to predict the Li-related isotope shifts. Li-related isotope shifts for OD are predicted to be only 0.3 % and 25% of the experimental value, respectively, for structures (b) and (a). Structure (c), the bond-centered structure, is favored both by its stability and by a predicted Li-related isotope shift for OD of 76% of the experimental value.
1. L. E. Halliburton *et al.*, J. Appl. Phys. **96**, 7168 (2004). 2. M. G. Wardle *et al.,* Phys. Rev. B **71**, 155205 (2005). 3. V. R. Saunders *et al., Crystal2003 User's Manual*, University of Torino, Torino, 2003.

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