

Abstract Submitted
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Vibrational properties of a Li – OH complex in ZnO¹ K. R. MARTIN, Lehigh University, University of Pittsburgh at Johnstown, P. M. BLANEY, G. A. SHI, M. STAVOLA, W. B. FOWLER, Lehigh University — Considerable interest has developed on the potential use of II-VI oxides as electronic and optical materials. In several cases alkali atoms have been suggested as dopants. We report on the theoretical and experimental investigation of infrared and vibrational properties of a Li-OH complex in ZnO. Earlier infrared experiments[1] revealed a broad OH-like band centered at 3577.3 cm^{-1} (12K), with full width at half maximum ranging from 0.4 cm^{-1} (12K) to 41.3 cm^{-1} (300K) and a corresponding shift in peak position of -29 cm^{-1} , suggesting a significant coupling of the OH stretch with other modes. We have performed similar experiments on the OD version of this defect and have theoretically investigated[2,3] the coupling of these stretch modes to other modes. The lack of a significant isotope dependence of the resulting parameters suggests that the defect couples to the host rather than the large-amplitude motion of the H or D itself. 1. L. E. Halliburton *et al.*, J. Appl. Phys. **96**, 7168 (2004). 2. B. N. J. Persson and R. Ryberg, Phys. Rev. B **32**, 3586 (1985). [3] M. Budde *et al.*, Phys. Rev. B **63**, 195203 (2001).

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