Vibrational properties of a Li – OH complex in ZnO

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 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 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.


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