

Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Unambiguous identification of an OH-Li center in ZnO: Experiment G.A. SHI, M. STAVOLA, W.B. FOWLER, Lehigh University — Theory has found that isolated H is always a donor in ZnO [1] and has led to a number of studies of the properties of H in this promising wide bandgap semiconductor. Of interest here is an OH vibrational line at 3577.3 cm^{-1} that is dominant in ZnO grown by the hydrothermal method [2,3]. We show that the two naturally abundant isotopes of Li [${}^6\text{Li}$ (7.5%) and ${}^7\text{Li}$ (92.5%)] cause the D-stretching counterpart of the 3577.3 cm^{-1} IR line to be split into two components that can be separately resolved, even though the 3577.3 cm^{-1} line itself shows no Li-related splitting. This unexpected result establishes unambiguously that the 3577.3 cm^{-1} IR line is due to an OH-Li complex. Overtone and oxygen isotope data for the OH-Li center provide an unusually complete picture of the vibrational properties of this defect. Because isotope splittings for elements heavier than Li will be more difficult to detect, this OH-Li center may be considered a model system for H trapped by impurities in ZnO.

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Date submitted: 26 Nov 2005

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