

Shallow Donor States Induced by In-Diffused Cu in ZnO: A Combined HREELS and Hybrid DFT Study

Hengshan Qiu,¹ Federico Gallino,² Cristiana Di Valentin,^{2,*} and Yuemin Wang^{1,†}

¹*Department of Physical Chemistry I and Laboratory of Industrial Chemistry, Ruhr University Bochum, D-44780 Bochum, Germany*

²*Dipartimento di Scienza dei Materiali, Università di Milano-Bicocca, 20125 Milano, Italy*

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A combined experimental and first principles study of Cu defects in bulk ZnO is presented. Cu particles are epitaxially deposited on the polar O-ZnO(000 $\bar{1}$) surface at room temperature. Upon heating, a broadening of the quasielastic peak in high resolution electron energy loss spectra is observed, corresponding to an electronic doping effect of Cu atoms in bulk ZnO with an ionization energy of 88 meV. Cu impurities in ZnO, although commonly acting as acceptors, are presently observed to induce shallow donor states. We assign these to interstitial Cu species on the basis of a hybrid density functional study.