Theoretical study of Si in ZnO

JOHN LYONS, ANDERSON JANOTTI, CHRIS VAN DE WALLE, Materials Department, University of California, Santa Barbara, CA 93106-5050 — Recently, the presence of silicon in relatively high concentrations has been detected in samples of ZnO [1]. The properties of this impurity have not yet been investigated. Here we present a first-principles study of the electronic and structural properties of Si in zinc-blende ZnO using density functional calculations with LDA, GGA, and hybrid functionals. Our calculations show that substitutional Si on a Zn site is lower in energy than either Si on an oxygen site or a Si interstitial. The calculations consistently predict Si to be a shallow donor in ZnO, with the 2+ charge state being most stable across the band gap. The formation energy of substitutional Si is relatively low, supporting experimental evidence which shows a concentration of $10^{17}$ cm$^{-3}$ Si in ZnO samples. The properties of Ge in ZnO are also studied for comparison and show behavior similar to that of Si. [1] M.D. McCluskey and S.J. Jokela, Physica B 401-402, 355 (2007).

$^1$Work supported by the NSF MRSEC Program under Grant No. DMR05-20415 and by the UCSB Solid State Lighting and Energy Center.