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Theoretical study of Si in ZnO[1] 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).

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