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Theory of copper impurities in ZnO[1] JOHN LYONS, Naval Research Laboratory, AUDRIUS ALKAUSKAS, Center for Physical Sciences and Technology, Vilnius, Lithuania, ANDERSON JANOTTI, Department of Materials Science and Engineering, University of Delaware, CHRIS G. VAN DE WALLE, Materials Department, University of California, Santa Barbara — Due to its connection to deep luminescence signals and its potential use as an acceptor dopant, copper has been one the most studied impurities in ZnO. From experiment, copper incorporating on the Zn site (CuZn) is known to lead to an acceptor level residing near the conduction band of ZnO, making CuZn an exceedingly deep acceptor. CuZn in ZnO has also long been linked with broad 2.4 eV green luminescence (GL) signals. In this work we explore the electrical and optical properties of Cu in ZnO using density functional theory (DFT). Due to the limitations of traditional forms of DFT, an accurate theoretical description of the electrical and optical properties of such deep centers has been difficult to achieve. Here we employ a screened hybrid density functional (HSE) to calculate the properties of Cu in ZnO. We determine the thermodynamic transition levels associated with CuZn in ZnO as well as the associated luminescence lineshapes [1] of characteristic optical transitions. We find that HSE-calculated optical transitions are in close agreement with experimental studies. [1] A. Alkauskas, J. L. Lyons, D. Steiauf, and C. G. Van de Walle, Phys. Rev. Lett. 109, 267401 (2012).

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