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DFT Study on ZnO Nanoplate Towards Magnetic Property SEUNG SOON JANG, JI-IL CHOI, JUNG-IL HONG, ZHONG LIN WANG, ROBERT SNYDER, Georgia Institute of Technology, School of Materials Science and Engineering — Using a GGA+U method and Density Functional Theory, we present a theoretical study for the existence of a magnetic moment in ZnO nanoplate without any extrinsic doping of magnetic impurities. Nanoplate are configured with a Zn-terminated (0001) surface and O-terminated $(000\bar{1})$ surfaces. The surface reconstruction was considered by optimizing the structures. Using GGA PBE, we calculated the spin density of states for both spin states and individual density of states for each orbital to clarify the degree of contributions. Compared to the electronic configuration of bulk wurtzite ZnO, net spins are observed in ZnO nanoplates depending on the plate thickness, which is thought to be due to large changes in the degree of hybridization throughout the plate. As the electronic configuration of a ZnO nanoplate is converged to that of bulk ZnO with increasing plate thickness, its net spin disappears. Specifically, It is found that the net spin of the ZnO nanoplate disappears when its thickness increases beyond $\sim$ 6 nm. In our presentation, we will discuss the change of the electronic configurations as a function of the plate thickness with a rationalization of this change.

Seung Soon Jang
Georgia Institute of Technology, School of Materials Science and Engineering

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