

Abstract Submitted  
for the MAR10 Meeting of  
The American Physical Society

**Size-dependent induced magnetism in carbon-doped ZnO nanostructures**<sup>1</sup> HYUNWOOK KWAK, Washington State University, JAMES CHELIKOWSKY, University of Texas — The role of quantum confinement on the carbon doped ZnO nanocrystals will be examined using a real-space, first-principles method. We find that the spin polarization energy of carbon defects in nanocrystals is sensitive to size owing to the partial occupancy of a less-localized minority spin state. In addition, we find that the partial occupancy of a minority spin state results in a direct exchange mechanism between the carbon defects even under strong confinement. The analysis suggests that the semiconductor with non-magnetically induced magnetic moments should provide a significant advantage over the traditional dilute magnetic semiconductors when applied to nanometer-scaled applications.

<sup>1</sup>The work was supported by the U. S. Department of Energy under DE-FG02-06ER15760. Computational resources were provided by the National Energy Research Scientific Computing Center and the Texas Advanced Computing Center.

Hyunwook Kwak  
Washington State University

Date submitted: 18 Nov 2009

Electronic form version 1.4