Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Achieving Room-temperature Ferromagnetism in N-doped ZnO with Inhomogeneity VIVIAN TRAN, Department of Materials Science and Engineering, University of California, Berkeley; and Graduate School of Engineering Science, Osaka University, MASAYOSHI SEIKE, TETSUYA FUKUSHIMA, KAZUNORI SATO, HIROSHI KATAYAMA-YOSHIDA, Graduate School of Engineering Science, Osaka University — Wide-gap semiconductors, such as ZnO, are attractive host materials for dilute magnetic semiconductors (DMS) due to potential applications in optoelectronic and magneto-optical devices. Recent experiments on N-doped ZnO DMS have reported room-temperature ferromagnetism (RTFM) under a homogeneous distribution of N-dopants. However, analogies to the previously studied transition-metal-doped ZnO systems suggest that RTFM originates from inhomogeneity in the system. Through first-principles calculations, we show that the N-dopants tend to cluster and that RTFM in N-doped ZnO DMS can be achieved by controlling the inhomogeneity in the system. That is, Monte Carlo simulations indicate that self-organized N-rich nanostructures form under layer-by-layer growth conditions. Furthermore, our calculations show that these nanostructures have strong ferromagnetic coupling between N-atoms within each nanostructure in addition to high blocking temperature, assuming a homogeneous distribution of dopants within each nanocluster. These self-organized nanostructures have potential applications to high-density magnetic memory.

Vivian Tran
University of California, Berkeley

Date submitted: 09 Nov 2012 Electronic form version 1.4