Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

**Defect Creation and Annihilation in GaN and ZnO**[1] CHRIS VAN DE WALLE, ANDERSON JANOTTI, University of California, Santa Barbara — ZnO is an extremely attractive material for a number of optoelectronic and electronic applications. Among its advantages is its radiation hardness, which is even greater than that of GaN. Based on our comprehensive investigations of intrinsic point defects [1,2], we have developed a model for defect creation and annihilation during and after irradiation. The calculations, based on pseudopotential-density-functional theory combined with LDA+U [2] produce formation energies, stability of charge states as a function of Fermi level, and migration barriers for each of the point defects. Migration barriers allow us to determine annealing temperatures at which we predict various defects to be mobile. In ZnO, the key factors responsible for radiation hardness are (1) the low migration barriers of point defects and (2) the charge-state matching of dominant defect pairs. Quantitative arguments for both ZnO and GaN will be presented, and the results compared with experimental observations. The insights provided by our modeling can be fruitfully applied to understand irradiation effects in semiconductors and insulators in general. [1] S. Limpijumnong and C. G. Van de Walle, Phys. Rev. B 69, 035207 (2004). [2] A. Janotti and C. G. Van de Walle, Phys. Rev. B 76, 165202 (2007).

[1]Work supported by the NSF MRSEC Program under award No. DMR05-20415.

Chris Van de Walle
University of California, Santa Barbara

Date submitted: 21 Nov 2008 Electronic form version 1.4