Abstract Submitted for the MAR07 Meeting of The American Physical Society

Mechanism of ferromagnetism in wide band gap semiconductors

PRIYA MAHADEVAN, S.N. Bose National Centre for Basic Sciences — Several wide bandgap semiconductors/oxides doped with small concentrations of transition metal impurities have been found to exhibit ferromagnetism at temperatures higher than room temperature. As the typical dopant concentrations are far below the percolation threshold associated with nearest neighbor cation coupling, a picture of ferromagnetism has been proposed which attributes an important role played by the intrinsic defects which are present in these materials. We have considered several examples of the most common defects found in GaN and ZnO, and examined within ab-initio calculations how their presence modifies ferromagnetism. Some defects, such as Ga-vacancies in GaN favor strongly spin polarised configurations with exchange splittings as large as 1 eV. However, the exchange splittings are quenched if the defect induced levels are below the transition-metal induced levels. We consider various scenarios for the location of the defect induced levels and the transition metal levels and identify the regime of defect enhanced ferromagnetism and examine various features of this regime.

Priya Mahadevan S.N. Bose National Centre for Basic Sciences, Kolkata, India

Date submitted: 16 Nov 2006 Electronic form version 1.4