Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Complexities in diluted magnetic semiconductors-a theoretical perspective from ab-initio electronic structure calculations BIPLAB SANYAL, DIANA IUSAN, OLLE ERIKSSON, Department of Physics, Uppsala University, Sweden — Diluted magnetic semiconductors (DMS), the essential materials for semiconductor spintronics, show a variety of complex properties, e.g., defect-mediated (ferro/antiferro)magnetic interactions and the disorder leading to magnetic percolation effects. Using the ab-initio Korringa-Kohn-Rostoker-Coherent-Potential-Approximation, the magnetic pair exchange parameters of a Heisenberg model have been calculated for Mn doped ZnO and half-Heusler NiTiSn hosts followed by the calculation of transition temperatures using Monte-Carlo simulations. Zinc vacancies and nitrogen substituting oxygen atoms lead to ferromagnetic interactions in Mn doped ZNO while in a defect free case, the interaction between Mn atoms is antiferromagnetic. The calculated critical temperatures are low ($\sim$35 K) due to the short-ranged exchange interactions and low defect concentration. In the other case, Mn doped NiTiSn shows a high critical temperature ($\sim$300 K) for 22 % Mn concentration. Below 3% Mn, there is no magnetic long range order as the magnetic percolation is not established. The results are in good agreement with experiments.

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Date submitted: 20 Nov 2006 Electronic form version 1.4