Spin waves in Mn-doped Si: exchange interactions from first-principles calculations G. Rao and J. E. Raynolds College of Nanoscale Science and Engineering, University at Albany, State University of New York

GAYATHRI RAO, JAMES RAYNOLDS, CNSE, University at Albany — There has been considerable interest in magnetic semiconductors in recent years for potential applications in the field of spintronics. The present work was motivated by recent experimental achievement of above-room-temperature magnetism in Mn-doped silicon (Phys.Rev.B 71, 033302 (2005)). We present the results of Density Functional calculations that have been carried out to determine the strength of the distance-dependant exchange interaction in Mn-doped Si. The exchange interaction determines the energy difference between ferro-magnetic and anti-ferromagnetic spin configurations and as such it provides for a prediction of spin-wave velocities. Such spin waves, if they exist, are of interest in that they may provide means for transmitting spin-based information. Comparison of the relative energy differences between ferromagnetic and anti-ferromagnetic configurations for a series of Mn locations yielded the distance dependant exchange interaction J(R). Interestingly we find that the exchange interaction is negative (anti-ferromagnetic) for short and long distances and is positive (ferromagnetic) for intermediate distances. This talk will present these findings along with estimates of spin-wave velocities, densities of states, band structure and spin-density distributions.

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Date submitted: 15 Nov 2006