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Exchange interactions of DMS alloys in the GW approximation[1]

MARK VAN SCHILFGAARDE, Arizona State University

Dilute Magnetic semiconductors are a new but little understood class of materials, and in particular the origin of ferromagnetism in these materials. As we will show, the LSDA combined with the rigid-spin approximation fails to predict the observed magnetism in many of these materials, and a key question is whether the failing is due to the approximations made, or is something else going on? The best understood of DMS is zincblende $Mn_xGa_{1-x}As$, with $x\tilde{<}0.1$. Optimally grown thin films have been recently shown to exhibit conventional temperature-dependent magnetization behavior with $T_c \sim 170$K. Using a standard LDA linear-response technique the LSDA total energy is mapped analytically onto a Heisenberg hamiltonian, which is analyzed for random and partially ordered structures. Temperature-dependent properties were investigated using a form of the Cluster Variation method for the Heisenberg model. The calculated T_c is predicted to increase with x to x=15%, reaching T_c ∼250K. For still larger x, T_c is predicted to fall and turn antiferromagnetic when x>50%. Clustering and spin-orbit coupling are both found to reduce T_c. Thus in this case the theory falls in good agreement with observed values for low concentration. An analysis shows the Mn e_g levels are responsible for the antiferromagnetic contribution. We show that suitable short-period superlattices can minimize this contribution, thus signficantly enhancing T_c. Many other less well studied DMS alloys–particularly nitride and oxide compounds–have now been reported with T_c exceeding 300K. Several of these cases were investigated, and the LSDA linear-response predicts low T_c, typically $T_c < 100$K. Moreover, the LDA results for $Mn_xGa_{1-x}As$ at large x are at variance, with observed ferromagnetism in a quantum dot of MnAs in the zincblende phase[1]. To address validity of the LSDA+rigid approximation, a we present results from a recent implementation of self-consistent GW calculation of the spin susceptibility. As will be described GW alters the exchange parameters in even in elemental transition metals, and the changes in transition metal compounds can be dramatic. [1]K. Ono et al, J. Appl. Phys. **91**, 8088 (2002).

[1]In collaboration with Takao Kotani. Supported by the Office of Naval Research