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Tailoring Magnetism in Bulk Semiconductors and Quantum Dots[1]

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Carrier-mediated magnetism in semiconductors shows important and potentially useful differences from their metallic counterparts [1]. For example, in magnetically doped semiconductors the change in carrier density induced by light or bias could be sufficient to turn the ferromagnetism on and off. However, there remain many important challenges to fully understand these materials. Our density functional theory study of Mn- doped II-IV-V_2 chalcopyrites [2] reveals that variation of magnetic properties across 64 different materials cannot be explained by the dominant models of ferromagnetism in semiconductors. We observe no qualitative similarity with the suggested Curie temperature scaling with the inverse cube of the lattice constant [3]. In contrast to most of the theoretical studies, we explicitly include the temperature dependence of the carrier density and propose a model which permits analysis of the thermodynamic stability of the competing magnetic states [4]. As an example we analyze the stability of a possible reentrant ferromagnetic semiconductor and discuss the experimental support for this prediction. An increasing temperature leads to an increased carrier density such that the enhanced coupling between magnetic impurities results in the onset of ferromagnetism as temperature is raised. We also use the real space finite-temperature local spin density approximation to examine magnetically doped quantum dots in which the interplay of quantum confinement and strong Coulomb interactions can lead to novel possibilities to tailor magnetism. We reveal that, even at a fixed number of carriers, the gate induced changes in the screening [5] or deviations from isotropic quantum confinement [6] could allow for a reversible control of magnetism and switching between zero and finite magnetization. Such magnetic quantum dots could also provide versatile voltage-control of spin currents and spin filtering. The work done in collaboration with S. C. Erwin (Naval Research Lab), A. G. Petukhov (South Dakota School of Mines and Technology), R. M. Abolfath (SUNY Buffalo) and P. Hawrylak (NRC, Canada).

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