Understanding the spin-glass state through the magnetic & electronic properties of Mn-doped ZnTe

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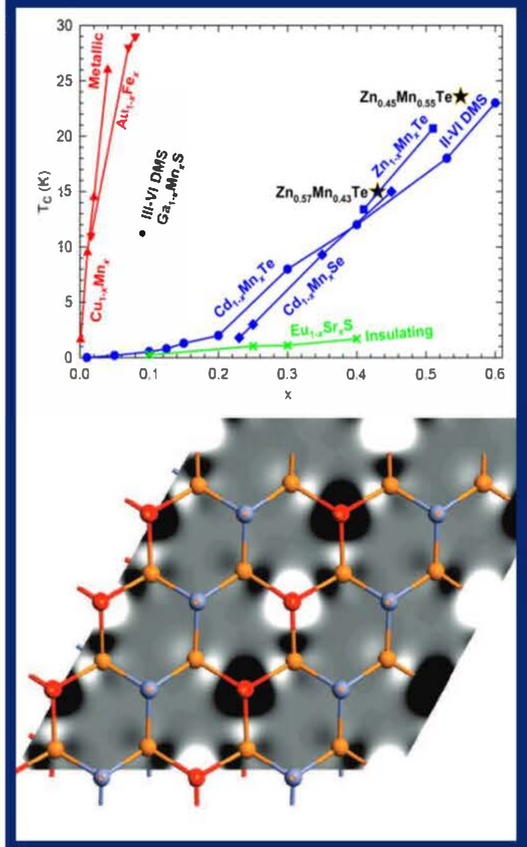
ABSTRACT:

To gain insight into the spin-glass state of diluted magnetic semiconductors, we have examined the magnetic and electronic properties of Mn-doped ZnTe using density functional theory. Using a generalized gradient approximation, we investigate the electronic and magnetic properties for x=0, 0.25, and 0.50 doping levels using the magnetic moment of Mn2+ as guide for the dependence of the Hubbard onsite potential on the electronic structure as well as a geometry optimization to assure an anti-ferromagnetic (AFM) ground state which is consistent with a zero magnetic moment spin glass state. An onsite potential of up to 8 eV on the Mn 3d-orbitals is needed to harden the magnetic moment toward S = 5/2. From our analysis of the electronic structure evolution with doping and onsite potential, we confirm the semiconducting state of the Mn-doped ZnTe as well as show that the presence of Mn incorporated into the ZnTe matrix at the Zn lattice site produces magnetic interactions through the Te ions with a distinct Te-Mn pd-orbital hybridization. Furthermore, we show that this hybridization is activated with the Mn doping above 25%, which corresponds to the doping level in which the spin-glass transition begins to rise. Therefore, it is likely that the coupling of pd-orbital hybridization of the Mn and Te p-orbitals is a precursor to the spin-glass state.

METHODS:

The *ab-initio* calculations are performed through density functional theory by using the atomistic orbital approach implemented in Quantum Atomistix Toolkit (QuantumATK). Calculations are carried out within the spin-polarized generalized gradient approximation (SGGA) to the exchange-correlation functional (PBE) with a variable onsite potential. Hubbard U was used to assure the ground state magnetic moment of spin 5/2. Magnetization measurements (not shown) were performed using a Quantum Design MPMS XL7 superconducting quantum interference device (SQUID) magnetometer.

The spin-glass nature of the Mn-doped ZnTe is produced through the magnetic exchange interactions and mediated by a *p*- and *d*- orbital hybridization.



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