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

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ABSTRACT:

To understand the spin-glass state of diluted magnetic semi-conductors, we have examined the magnetic properties of $Zn_{1-x}Mn_xTe$ using density functional theory and magnetization measurements. Utilizing the generalized gradient approximation, we investigate the dependence of the Hubbard onsite potential on the magnetization and electronic structure. We find that the ground state magnetic preference is antiferromagnetic and that the onsite potential is needed to harden the magnetic moment of S = 5/2. Furthermore, the system is clearly semi-conducting, which suggests that the spin-glass nature of the compound is produced through the magnetic exchange interactions through the *p*- and *d*-orbital hybridization.

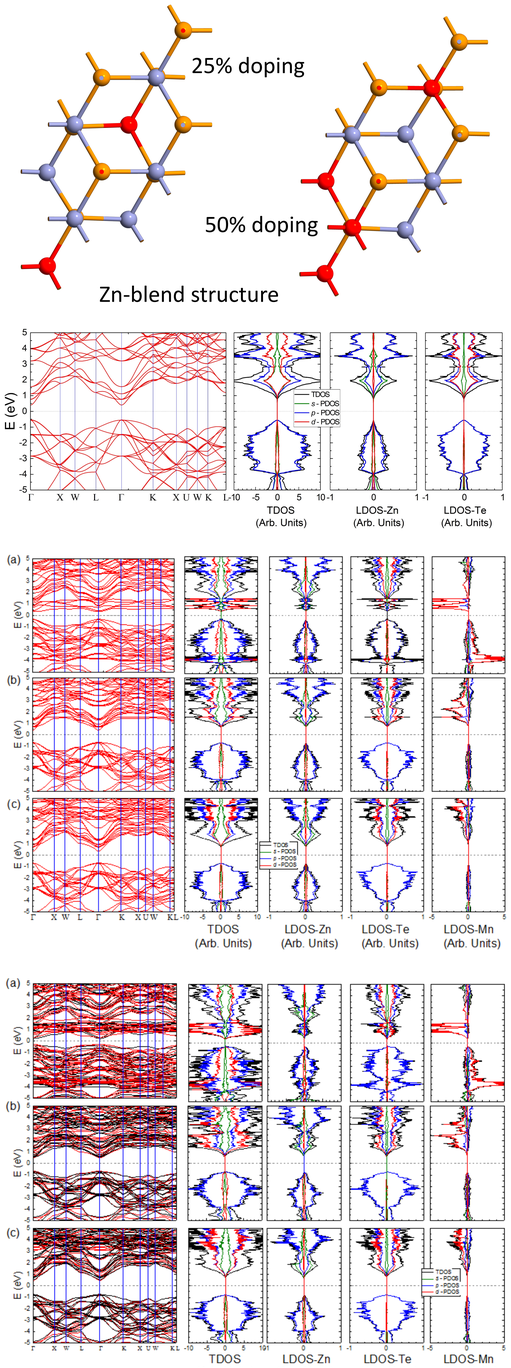
METHODS:

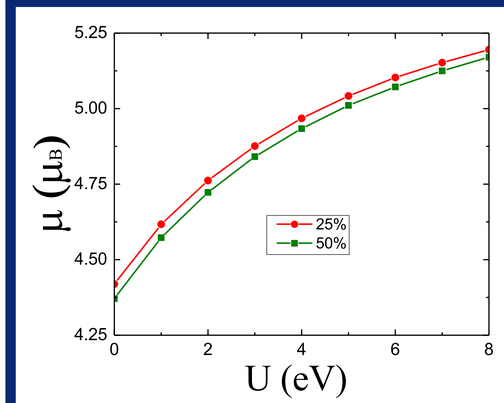
The *ab-initio* calculations are performed based on the density functional theory by using the atomistic orbital approach implemented in Quantum Atomistix Toolkit (QuantumATK). Calculations are carried out within the spin-polarized generalized gradient approximation (SGGA) to the exchange-correlation functional (PBE) with a variable onsite potential. The 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.

CONCLUSIONS:

Using magnetization measurements and density functional theory, we find that the spin state of Mn-doped ZnTe is consistent with the stoichiometric value of spin 5/2. Furthermore, with this value, the electronic and optical properties are reproduce the proper gap value.

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





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