

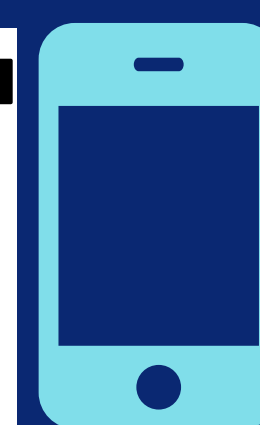
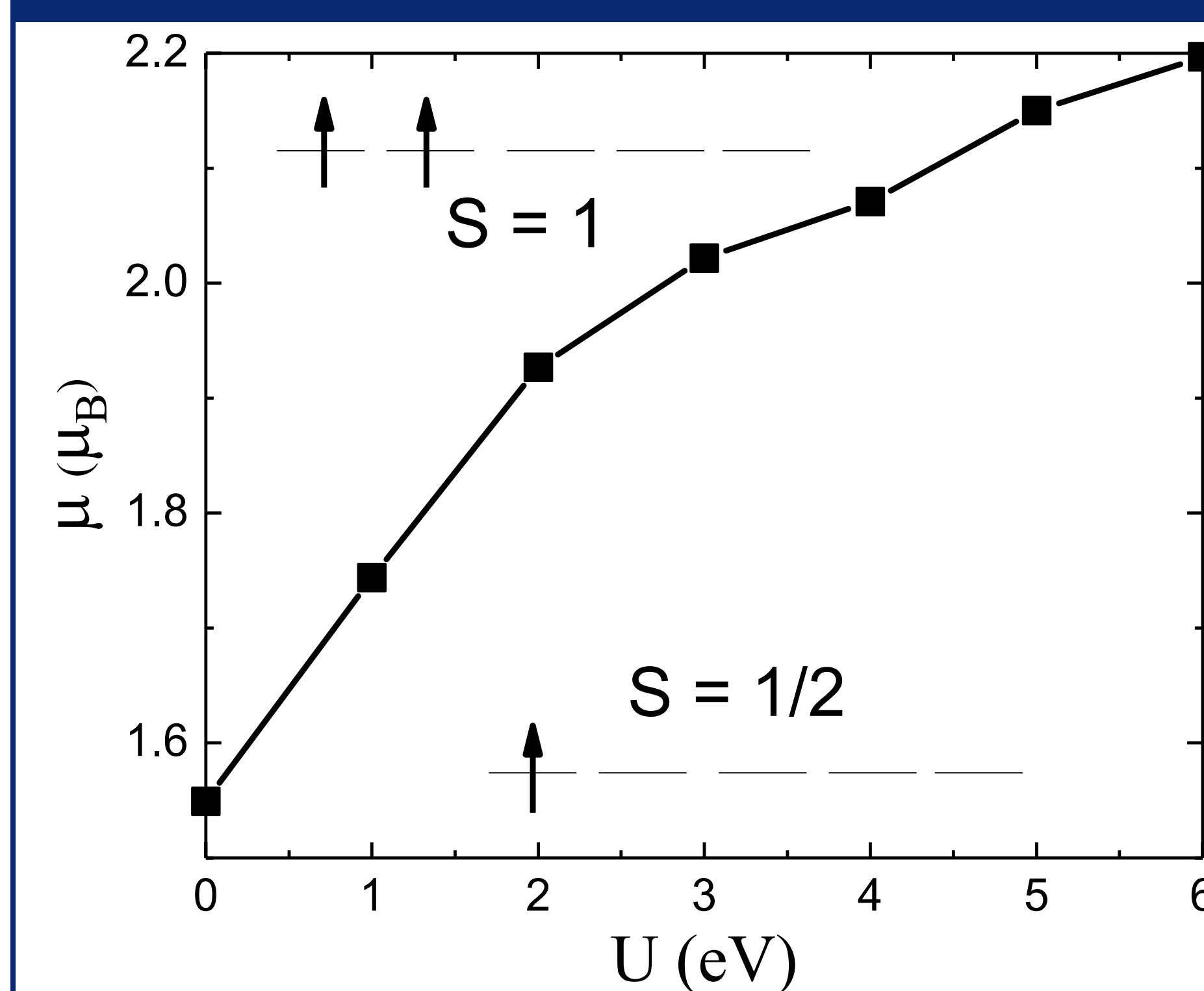
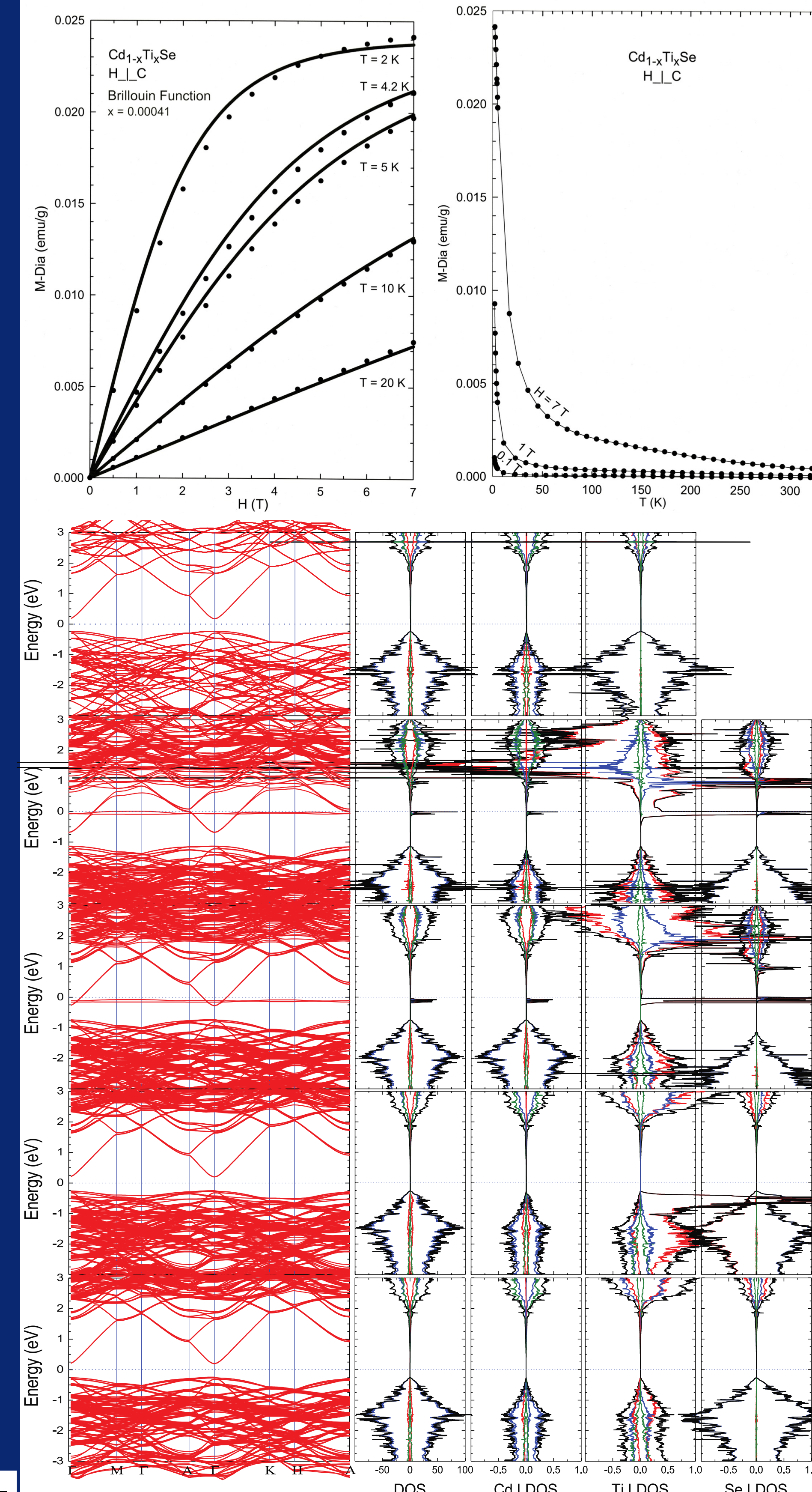
ABSTRACT:

Using computational and experimental techniques, we examine the nature of the 2+ oxidation of Ti-doped CdSe. Through stoichiometry and confirmed through magnetization measurements, the weakly-doped material of $\text{Cd}_{1-x}\text{Ti}_x\text{Se}$ ($x = 0.0043$) shows the presence of a robust spin-1 magnetic state of Ti, which is indicative of a 2+ oxidation state. Given the obscure nature of the Ti^{2+} state, we investigate the electronic and magnetic states using density functional theory. Using a generalized gradient approximation with an onsite potential, we determine the electronic structure, magnetic moment density, and optical properties for a supercell of CdSe with an ultra-low concentration of Ti. We find that, in order to reproduce the magnetic moment of spin-1, an onsite potential of 4-6 eV must be included in the calculation. Furthermore, the electronic structure and density of states shows the presence of a Ti-d impurity band above the Fermi level and a weakly metallic state for a $U = 0$ eV. However, the evolution of the electronic properties as a function of the Hubbard U shows that the Ti-d drop below the Fermi around 4 eV with the onset of a semiconducting state. The impurity then mixes with the lower valence bands and produces the 2+ state for the Ti atom.

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.

The onset of the semiconducting state induces a shift in the valence levels and produces the localization of the second spin in the d -band and the spin-1 state



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