

Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

On the Electronic and Magnetic Properties of the ionic superatomic solid $\text{Ni}_9\text{Te}_6(\text{PEt}_3)_8\text{C}_{60}$ ¹ VIKAS CHAUHAN, SANJUBALA SAHOO, SHIV KHANNA, Virginia Commonwealth University, PHYSICS DEPARTMENT VCU COLLABORATION — We have carried out first principles electronic structure studies to examine the atomic structure, stability, and electronic and magnetic properties of the recently synthesized $\text{Ni}_9\text{Te}_6(\text{PEt}_3)_8\text{C}_{60}$ ionic material consisting of $\text{Ni}_9\text{Te}_6(\text{PEt}_3)_8$ superatoms and C_{60} . It is shown that the PEt_3 ligands result in an internal coulomb well that lifts the quantum states of the Ni_9Te_6 cluster lowering its ionization potential to 3.39 eV thus creating a superatomic alkali motif. The metallic core has a spin magnetic moment of 5.3 μ_B in agreement with experiment. The clusters are marked by low magnetic anisotropy energy (MAE) of 2.72 meV and a larger intra-exchange coupling exceeding 0.2 eV indicating that the observed paramagnetic behavior around 10K is due to superparamagnetic relaxations. The magnetic motifs separated by C_{60} experience a weak superexchange that stabilizes a ferromagnetic ground state as observed around 2K. The calculated MAE is sensitive to the charged state that could account for the observed change in magnetic transition temperature with size of the ligands or anion.

¹We gratefully acknowledge funding support from the Department of Energy under Award Number DE-SC0006420.

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Date submitted: 06 Nov 2015

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