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**Modeling of Magnetic Behavior of Superatomic-Fullerene Assemblies** PALLABI SUTRADHAR, VIKAS CHAUHAN, SHIV N. KHANNA, JAYASIMHA ATULASIMHA, Virginia Commonwealth University — We recently carried out theoretical studies [1] on recently synthesized magnetic superatomic solids [2], consisting of magnetic $Ni_9Te_6(Pet_3)_8$ clusters separated by non-magnetic $C_{60}$. We studied the magnetic response of the superatomic solid by constructing the Hamiltonian for a small assembly of metal clusters interacting through the fullerene by including isotropic and anisotropic exchange interactions, magnetic anisotropy energy and Zeeman energy for the interaction between the cluster magnetic moment and the global magnetic field. Furthermore, we showed that inclusion of Dzyaloshinskii-Moriya interaction that causes spin canting was essential in order to explain the experimental trend. Here we will extend this analysis to study the magnetic response of larger Superatomic-Fullerene assemblies (supersolids) through Monte Carlo simulations to understand temperature and size effects. [1] P. Sutradhar et al., Phys. Chem. Chem. Phys., 2016 (Selected for highlight on back cover) DOI: 10.1039/c6cp05196k. [2] C.H. Lee et al., J. Am. Chem. Soc. 136, 16926, 2014.
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