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Computational Atomistic Modeling of Bi-Magnetic Core-Shell Nanoparticles[1] RAHUL SAHAY, Sacred Heart Academy and Department of Physics, Central Michigan University, Mount Pleasant, MI, JUAN PERALTA, Department of Physics, Central Michigan University, Mount Pleasant, MI, 48859, GABRIEL CARUNTU, Department of Chemistry, Central Michigan University, Mount Pleasant, MI, 48859 — Since its discovery, there has been an increasing interest in the modeling of magnetic phenomena found in materials that present exchange bias. In particular, ferro-antiferromagnetic core-shell nanoparticles are an interesting case in which the magnetic properties of the nanostructure can be altered by adjusting their size, shape, and composition. Here we present a computational scheme that efficiently models the magnetic behavior of bi-magnetic core-shell nanostructures. Using a Heisenberg-Dirac-van Vleck Hamiltonian in combination with a continuous spin model, we simulate a wide range of hysteresis diagrams displaying exchange bias. Furthermore, we will demonstrate our efforts towards improving the efficiency of the simulation algorithms, aiming to afford magnetic atomistic simulations of large nanostructures by using a method based on a tessellated unit sphere to account for spin orientations. Our results allow for further semi-quantitative comparisons with existing experimental data and provide a means to discover new phenomena associated with these core-shell nanoparticles and other nanostructures.

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