Abstract Submitted
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A Hybrid DFT Description of the Ground State Properties of Americium-I[1] RAYMOND ATTA-FYNN, ASOK RAY, Physics Department, The University of Texas at Arlington — Americium-I (Am-I) is a strongly correlated metal which has been determined experimentally to be a non-magnetic, double HCP crystal with well-localized $5f$ electrons. However, theoretical descriptions of Am-I based on density functional theory (DFT) yield the correct structural properties but the wrong magnetic ground state and a very poorly described $5f$ electron spectra. In this work, we will show that hybrid DFT, which replaces a fraction (40% to be exact) of approximate DFT exchange with exact Hartree-Fock (HF) exchange, yields structural, magnetic, and electronic properties of Am-I which are in excellent agreement with experimental data. The primary reason why DFT fails to describe Am-I, namely the overestimation of the exchange interaction leading to a spin-polarized ground state, and how this failure is corrected by hybrid DFT, will be discussed.

[1]R. Atta-Fynn and A. K. Ray, Chemical Physics Letters, **482**, 223-227 (2009). This work is supported by the U. S. Department of Energy and the Welch Foundation, Houston, Texas.

Raymond Atta-Fynn
Physics Department, The University of Texas at Arlington

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