

Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Magnetic and thermodynamic properties of Americium-II: An *Ab Initio* Study¹ JIANGUANG WANG, LI MA, ASOK RAY, University of Texas at Arlington — Hybrid density functional theory based method has been used to study the structural, magnetic, electronic, and thermodynamic properties of Americium-II. Non-magnetic, ferromagnetic (FM), and anti-ferromagnetic (AFM) configurations without and with spin-orbit coupling (SOC) have been considered. The experimental NM ground state configuration is indeed obtained for Am-II at a level of 40% HF exchange with SOC and the computed structural properties and electronic density of states are in good agreement with experimental observations. The importance of SOC is found to be significant. The phonon related properties of Am-II are presented for the NM ground state configuration and the computed heat capacity and entropy are in good agreement with the experimental measurements. The lattice constant, bulk modulus, heat capacity, and entropy of Am-II are predicted to be 9.44 a.u., 21.7 GPa, 24.3 JK⁻¹mol⁻¹, and 55.7 JK⁻¹mol⁻¹, respectively.

¹This work is partially supported by the Welch Foundation, Houston, Texas (Grant No. Y-1525) and by the Department of Energy.

Jianguang Wang
University of Texas at Arlington

Date submitted: 13 Nov 2010

Electronic form version 1.4