Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Electronic and thermodynamic properties of layered Hf_2S from first-principles calculations CHANDANI NANDADASA, Mississippi State University; Oak Ridge National Laboratory, MINA YOON, Oak Ridge National Laboratory, SEONG-GON KIM, Mississippi State University, STEVE ERWIN, Naval Research Laboratory, SUNGHO KIM, SUNG WNG KIM, Sungkyunkwan University, KIMOON LEE, Kunsan National University — Theoretically we explored two stable phases of inorganic fullerene-like structure of the layered dihafnium sulfide (Hf_2S). We investigated structural and electronic properties of the two phases of Hf_2S by using first-principles calculations. Our calculation identifies experimentally observed anti- NbS_2 structure of Hf_2S. Our electronic calculation results indicate that the density of states of anti- NbS_2 structure of Hf_2S at fermi level is less than that of the other phase of Hf_2S. To study the relative stability of different phases at finite temperature Helmholtz free energies of two phases are obtained using density functional theory and density functional perturbation theory. The free energy of the anti- NbS_2 structure of Hf_2S always lies below the free energy of the other phase by confirming the most stable structure of Hf_2S. The phonon dispersion, phonon density of states including partial density of states and total density of states are obtained within density functional perturbation theory. Our calculated zero-pressure phonon dispersion curves confirm that the thermodynamic stability of Hf_2S structures. For further investigation of thermodynamic properties, the temperature dependency of thermal expansion, heat capacities at constant pressure and volume are evaluated within the quasiharmonic approximations (QHA).

Chandani Nandadasa
Mississippi State University

Date submitted: 23 Nov 2016 Electronic form version 1.4