

Abstract Submitted
for the SHOCK05 Meeting of
The American Physical Society

High Pressure & High Temperature Equation of State and Magnetic Phase Transitions of Hematite from First Principles SATHYA HANAGUD, XIA LU, Georgia Institute of Technology — α -Fe₂O₃ (Hematite) is of special interest in the design of multifunctional structural energetic materials (SEM), based on a thermite mixture of metal and metal oxide. In this paper, from first-principles, we obtained the thermodynamically complete EOS $P = P(\rho, T)$ for hematite for pressures up to 50GPa and temperatures up to 1000K. There are only a few theoretical works on hematite. The difficulty of techniques traces back to the complication of the description of highly correlated d-electrons induced localization of valence states in Fe, and the mixing of the O 2p states and the Fe 3d states. In this paper, we implemented the ground state calculations in the framework of DFT, using sGGA and projector augmented wave approach. Particularly, the Hubbard-U method is used to describe the on-site Coulomb interactions of strongly correlated d-electrons in Fe atoms. The lattice thermal contributions are obtained by populating the phonon modes, according to the Boltzmann statistics. In comparison to the previous studies, the thermal contributions to EOS from lattice vibrations are included. In addition, we investigate the magnetic phase transitions at pressures and temperatures of interest. In the applications of SEMs, pressures are lower than 50 GPa which exclude the HP phases. The phonon dispersion curves with Hubbard-U are compared with those without Hubbard-U.

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Date submitted: 08 Apr 2005

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