Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Cohesion of $BaReH_9$ and $BaMnH_9$: Density Functional Calculations and Prediction of $(MnH_9)^{2-}$ Salts[1] DAVID SINGH, Oak Ridge National Laboratory, M. GUPTA, Universite Paris-Sud, R. GUPTA, CEA, Saclay — Density functional calculations are used to calculate the structural and electronic properties of $BaReH_9$ and to analyze the bonding in this compound. This compound has an exceptionally high H to metal ratio of 4.5. The high coordination of Re in $BaReH_9$ is due to bonding between Re 5d states and states of d-like symmetry formed from combinations of H s orbitals in the H_9 cage. This explains the structure of the material, its short bond lengths and other physical properties, such as the high band gap. We compare with results for hypothetical $BaMnH_9$, which we find to have similar bonding and cohesion to the Re compound. This suggests that it may be possible to synthesize $(MnH_9)^{2-}$ salts. Depending on the particular cation, such salts may have exceptionally high hydrogen contents, in excess of 10 weight %.

[1]Work at ORNL is supported by DOE, DMS&E.

David Singh
Oak Ridge National Laboratory

Date submitted: 30 Oct 2006 Electronic form version 1.4