Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Mercury Fluorides under high pressure: Hg as a pressure-induced transition metal JORGE BOTANA, XIAOLI WANG, Beijing Computational Science Research Center, Beijing 100084, P. R. China, DADONG YANG, Department of Physics, Beijing Normal University, Beijing 100875, P. R. China, HAIQING LING, Beijing Computational Science Research Center, Beijing 100084, P. R. China, YANGMING MA, State Key Lab of Superhard Materials, Jilin University, Changchun 130012, P. R. China, MAO-SHENG MIAO, Materials Department and Materials Research Laboratory, University of California, Santa Barbara, CA 93106-5050 — Hg has recently been found experimentally to be capable of forming a chemical compound, HgF_4, where it behaves as a transition metal, with an oxidation number of IV, but this molecule is very short lived. In this work we present theoretical evidence obtained through *ab initio* calculations that higher oxidation states than II can be stabilized in crystalline form for Hg, under extreme pressure. We have performed a structural search and optimization by means of Particle Swarm Optimization and Density Functional Theory for the crystalline series of HgF_n (n=3,4,5,6), and then used those data to draw the phase diagram of the equilibrium among those stoichiometries and HgF_2 and F_2. We have found that from 0 to 38 GPa only the mixture of HgF_2 and F_2 phases is thermodynamically stable. HgF_3 and HgF_4 have been found to be thermodynamically stable in different pressure ranges (from 73 GPa to at least 500 GPa and from 38 GPa to 200 GPa, respectively). We have also found that the HgF_3 crystal shows a very interesting band structure that suggests it could be a transparent conductor.

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Date submitted: 07 Nov 2013 Electronic form version 1.4