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Mercury Induced by Pressure to act as a Transition Metal in Mercury Fluorides JORGE BOTANA, Beijing CSRC, XIAOLI WANG, Institute of Condensed Matter Physics, Linyi University, CHUNJU HOU, School of Science, JiangXi University of Science and Technology, DADONG YAN, Department of Physics, Beijing Normal University, HAIQING LIN, Beijing CSRC, YANMING MA, State Key Lab of Superhard Materials, Jilin University, MAO-SHENG MIAO, Department of Chemistry and Biochemistry, California State University — The question of whether Hg is a transition metal remains open for stable solids. In our work we propose that high-pressure techniques will help prepare unusual oxidation states[1] of Hg in Hg-F compounds. By means of *ab initio* calculations and an advanced structure-search algorithm we find that under high pressure charge is transferred from the Hg d orbitals to the F, and becomes a transition metal.[2] HgF_3 and HgF_4 have been found to be stable compounds at high pressure. HgF_4 consists of planar molecules, a typical geometry for d^8 metallic centers. HgF_3 is an example of metallic and ferromagnetic compound, with an electronic structure analogous to transparent conductors due to the Hg d^9 configuration.

References

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