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Achieving unusual oxidation state of matter under high pressure

XIAOLI WANG, Beijing Computational Science Research Center Beijing, 100084, P. R. China Institute of Condensed Matter Physics, Linyi University Linyi 276005, P. R., HAIQING LIN, Beijing Computational Science Research Center Beijing, 100084, P. R. China, YANMING MA, State Key Lab of Superhard Materials, Jilin University Changchun 130012, P. R. China, MAOSHENG MIAO, Materials Research Lab, University of California Santa Barbara, CA 93110, USA — Pressure has many effects to matter including the reduction of the volume, the increase of the coordination number and the broadening of the band-widths. In the past, most of the high-pressure studies focused on structural and electronic state phase transitions. Using first principles calculations and a bias-free structural search method, we will demonstrate that high pressure can lead to high oxidation state of elements that can never be achieved under ambient condition, making high pressure technique a nice tool to explore many traditional topics in solid state and molecular chemistry. As an example, we will show that Hg can transfer the electrons in its outmost d shell to F atoms and form HgF_4 molecular crystals under pressure, thereby acting as a true transition metal. Group IIB elements, including Zn, Cd, and Hg are usually defined as post-transition metals because they are commonly oxidized only to the +2 state. Their d shells are completely filled and do not participate in the formation of chemical bonds. Although the synthesis of HgF_4 molecules in gas phase was reported before, the molecules show strong instabilities and dissociate. Therefore, the transition metal propensity of Hg remains an open question.

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