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Pressure makes mercury a transition metal: a first-principles study of HgF4 solid phases XIAOLI WANG, HAIQING LIN, Beijing Computational Science Research Center, YANMING MA, State Key Lab of Superhard Materials, Jilin University, MAOSHENG MIAO, Materials Research Lab, University of California Santa Barbara — Mercury is considered as a post-transition metal, because its d shell is filled and does not involve in forming chemical bonds. Yet, because the large relativistic effect pushes up the outmost d level, there is a high expectation that Hg can be stabilized in a higher oxidation state. The HgF4 molecule has been predicted by calculations, and an evidence of such molecule is shown by IR absorption recently. However, there is neither computation nor experiment report on possible high oxidation state of Hg in solid. By using first-principles density functional theory and a structure-searching method, we studied the structural change of a solid system of Hg and F under pressures from 0 to 300 GPa. We found that at lower pressure, the stable structure consists of HgF2 and F2 molecules. At about 25 GPa, the system undergoes a structural change and forms HgF4 planar molecules featuring d8 configuration. The calculations show that the d orbitals of Hg involve in chemical bonding, which is the signature of a transition metal.

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