Abstract Submitted
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Structure and Metallization of Hydrogen Iodide[1] STANIMIR BONEV[2], Lawrence Livermore National Laboratory, Livermore, CA 94550, VAHID ASKARPOUR, Department of Physics, Dalhousie University, Halifax, NS, Canada, B3H 3J5 — The structure and the metallization mechanism of hydrogen iodide under pressure are investigated using GW and hybrid density functional theory methods with exact exchange. The band gap closure is explained in terms of overlapping iodine p orbitals and a close correlation is shown to exist between evolving structural and electronic changes. The metallization transition in phase III of hydrogen iodide is determined to take place between 20 and 25 GPa at zero temperature. This result differs significantly from existing experimental data.

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