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Unusual Stoichiometries of Hydrogen and Iodine Under Pressure

ANDREW SHAMP, EVA ZUREK, University at Buffalo, SUNY — Evolutionary structure searches are combined with density functional calculations to examine the most stable stoichiometries and structures of hydrogen rich iodine phases, H_nI with n>1, under pressure. With respect to decomposition into hydrogen and iodine the first of the stoichiometries, H_5I, is predicted to become thermodynamically preferred at ∼30 GPa and remain stable until H_2I, consisting of chains of molecular hydrogen within a iodine sublattice, becomes the global thermodynamic minimum at ∼90 Gpa. H_5I consisting of both molecular and atomic hydrogen within H—I—H chains is predicted to remain insulating until ∼70 GPa whereas the H_2I stoichiometry is predicted to become metallic at ∼5GPa, well before it becomes thermodynamically stable. A second metallic phase, H4I, present on the convex hull at pressures above 100 GPa is constructed of a graphene-like molecular hydrogen sublattice between layers of a hexagonal iodine sublattice.

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