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Chemical Bonding Forces and Metallization of Hydrogen IVAN NAUMOV, RUSSELL HEMLEY, Carnegie Inst of Washington, CARNEGIE INST OF WASHINGTON COLLABORATION — Recent theoretical and experimental studies reveal that compressed molecular hydrogen at 200-350 GPa transforms to layered structures consisting of distorted graphene sheets. The new phases of dense solid hydrogen contrast with the long-held view that symmetric close-packed, ambient alkali-metal-like structures form at these high pressures –this raises the question about the nature and fate of molecular bonding in hydrogen on compression. The realization of such unexpected structures can be explained by consideration of simple low-dimensional model systems- H6 rings and graphene-like monolayers. Both molecular quantum chemistry and well-tested solid state approaches show that these model systems like aromatic hydrocarbons exhibit a special stability, associated with the completely filled set of bonding orbitals or valence bands. This close-shell effect persists in progressing to the real layered structures where it prevents the dielectric energy gap from closing, thus delaying the pressure-induced metallization. The latter nevertheless can occur upon further compression via destroying the closed shell electronic structure which is mainly determined by the 1s electrons. The most likely scenario is the lowering of the bonding bands (their bottoms) stemming from the unoccupied atomic 2s and 2p orbitals [1]. This research was supported by EFree, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award DESC0001057. [1] I. I. Naumov and R. J. Hemley, Acc. Chem. Res. 47, 3551-3559 (2014).

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