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Graphene physics and insulator-metal transition in compressed hydrogen[1] IVAN I. NAUMOV, R.E. COHEN, RUSSELL J. HEMLEY, Geophysical Lab, Carnegie Institution of Washington — As established recently both theoretically and experimentally, compressed hydrogen passes through a series of layered structures in which the layers can be viewed as distorted graphene sheets. These structures and their electronic properties can be understood by studying simple model systems-(i) a H_6 ring, (ii) an ideal single hydrogen graphene sheet and (iii) three-dimensional model lattices consisting of such sheets [1]. The energetically stable structures result from structural distortions of model graphene-based systems due to electronic instabilities towards Peierls or other distortions associated with the opening of a bandgap. Two factors play crucial roles in the metallization of compressed hydrogen: (i) crossing of conduction and valence bands in hexagonal or grapheme-like layers due to topology and (ii) formation of bonding states with $2p_z$ π character.

[1] I. I. Naumov, R. E. Cohen and R. J. Hemley Phys. Rev. B, **88**, 045125 (2013).

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Ivan I. Naumov
Carnegie Inst of Washington

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