Semimetallic and metallic states of crystalline molecular hydrogen

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The transition of molecular crystalline hydrogen from the semiconducting state to the semimetallic and metallic states has been discovered upon compression in the pressure range of 302—626 GPa along the 100 K isotherm.
At pressures below 361 GPa, the molecular crystal with the C2/c structure is a semiconductor with an indirect gap. Upon further compression, the indirect gap between the conduction and valence bands closes. In this case, the direct gap remains open. Thus, in the pressure range 361—527 GPa, the valence band is partially unoccupied, and the conduction band is partially filled, which indicates the semi-metallic nature of the conductivity. Moreover, the formation of a semi-metallic state is accompanied by a sharp increase in electrical conductivity in a narrow pressure range from 361 GPa to 389 GPa, which is in a good agreement with the experimental data. When compressed to pressures above 544 GPa, the structure changes from monoclinic C2/c to orthorhombic Cmca, accompanied by a sharp decrease (by more than two orders of magnitude) in the value of the direct gap, which is an indication of the metallic nature of the conductivity of the resulting structure. The resulting metallic state is metastable and exists up to a pressure of 626 GPa.
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