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Quasiparticle energies and excitonic effects of solid hydrogen under ultrahigh pressures ZHIGANG WU, MARC DVORAK, Colorado School of Mines, XAOJIA CHEN, Carnegie Institution of Science — We investigate the insulator-to-metal transition in the crucial *Cmca-12* phase of solid hydrogen employing the many-body perturbation theory with Green's functions. In particular quasiparticle energies are calculated within the *GW* approximation to accurately determine the insulator-to-metal transition pressure. We consider the effects of self-consistency, plasmon-pole models to the dielectric function, off-diagonal elements of the self-energy, and vertex corrections on *GW* calculations, and our results show that the band gap of the *Cmca-12* phase of solid hydrogen is sensitive to the choice of *GW* procedures and approximations involved, leading to a change of ~ 20 GPa in transition pressure. We also compute the optical absorption and electron-hole binding energy by solving the Bethe-Salpeter equation, and the resulting optical absorption shows a redshift and enhancement of absorption peaks compared to the GW-RPA absorption with excitonic effects omitted.

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