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Quasiparticle band structures of β-HgS, HgSe, and HgTe NIELS E. CHRISTENSEN, AXEL SVANE, Aarhus University, Denmark, MANUEL CARDONA, Max Planck Institute FKF, Stuttgart, ATHANASIOS CHANTIS, American Physical Society, MARK VAN SCHILFGAARDE, Arizona State University, Tempe, TAKAO KOTANI, Tottori University, Japan — The electronic structures of mercury chalcogenides in the zinc-blende strucrure have been calculated by the LDA, *GW* (one-shot, G_0W_0) and quasi-particle self-consistent *GW* (*QSGW*) approximations including spin-orbit coupling (SO). The slight tendency to overestimation of the band gaps by *QSGW* is avoided by using a *hybrid* scheme (20% LDA and 80 % *QSGW*. The results of G_0W_0 depend strongly starting wave functions and are thus quite different from those from *QSGW*. Within *QSGW* HgS is found to be a semiconductor, with a Γ_6 s-like conduction-band minimum state above the valence-band top Γ_7 and Γ_8 ("negative" SO splitting). HgSe and HgTe have "negative" gaps (inverted band structure). In HgTe the Γ_7 state is below Γ_6 due to the large Te SO splitting, in contrast HgSe where Γ_6 is below Γ_7.

Niels E. Christensen
Aarhus University

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