

Abstract Submitted  
for the MAR10 Meeting of  
The American Physical Society

**Quasiparticle band structures of PbS, PbSe and PbTe including pressure effects** AXEL SVANE, NIELS E. CHRISTENSEN, Aarhus University, Aarhus, Denmark, MANUEL CARDONA, Max Planck Institut FKF, Stuttgart, Germany — The electronic quasiparticle energies of PbS, PbSe and PbTe are calculated with the quasiparticle self-consistent GW approximation (QSGW, van Schilf-gaarde, Kotani and Faleev) including spin-orbit coupling. The semiconducting gap is formed between states of  $L_6$  symmetry ( $L_6^+$  and  $L_6^-$ ), which is the reason why these materials are semiconductors even in the local-density approximation (LDA) due to band repulsion. Closer inspection reveals that in PbS and PbSe the order of the  $L_6$  states is reversed in the LDA compared to the QSGW bands. This leads to the wrong sign of the band gap deformation potentials for PbS and PbSe in the LDA. With QSGW both sign and magnitude of the deformation potentials are in agreement with experiments. Also, results obtained for effective masses and band gaps as functions of pressure will be discussed.

N.E. Christensen  
Aarhus University

Date submitted: 12 Nov 2009

Electronic form version 1.4