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Analysis of core-valence linearization in G_0W_0 calculations RICARDO GOMEZ-ABAL, X. LI, M. SCHEFFLER, Fritz-Haber-Institute, Berlin, Germany, C. AMBROSCH-DRAXL, Materials Physics Department, University of Leoben, Austria — In recent years the GW approach, typically applied as the first order correction to the Kohn-Sham (KS) eigenenergies (G_0W_0 approximation), has substantially improved the description of single-particle excitations in weakly correlated semiconductors and insulators. Most of the existing codes are based on the pseudopotential (PP) method. It is well known from ground-state calculations that the linear treatment of the core-valence exchange-correlation interaction is not always valid. However, in the G_0W_0-PP scheme, the self-energy is computed from the (pseudo-)valence states only, keeping the core-valence interaction at the KS level. There is no justification for such a "core-valence linearization" of the dynamical self-energy, a highly non-linear functional of the total density. Nevertheless, G_0W_0-PP results usually agree better with experiments than the all-electron ones. In this talk we analyze the reasons for this disturbing discrepancy and the validity of the "core-valence linearization" in the G_0W_0-PP scheme. Calculations are performed using our own all-electron G_0W_0 code, based on the Wien2k implementation of the FP-(L)APW+lo method. We compare our all-electron results with those obtained by computing the self-energy from the valence states only as well as with G_0W_0-PP calculations for selected materials (e.g. Si, NaCl,...).

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