Efficient many-body calculations for two-dimensional materials using exact limits for the screened potential: Band gaps of MoS\(_2\), h-BN, and phosphorene - DTU Orbit (10/01/2019)

Calculating the quasiparticle (QP) band structure of two-dimensional (2D) materials within the GW self-energy approximation has proven to be a rather demanding computational task. The main reason is the strong \( q \) dependence of the 2D dielectric function around \( q = 0 \) that calls for a much denser sampling of the Brillouin zone (BZ) than is necessary for similar three-dimensional solids. Here, we use an analytical expression for the small \( q \) limit of the 2D response function to perform the BZ integral over the critical region around \( q = 0 \). This drastically reduces the requirements on the \( q \)-point mesh and implies a significant computational speedup. For example, in the case of monolayer MoS\(_2\), convergence of the \( G_0W_0 \) band gap to within similar to 0.1 eV is achieved with 12 x 12 \( q \) points rather than the 36 x 36 mesh required with discrete BZ sampling techniques. We perform a critical assessment of the band gap of the three prototypical 2D semiconductors, MoS\(_2\), h-BN, and phosphorene, including the effect of self-consistency at the GW\(_0\) level. The method is implemented in the open source code GPAW.

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