Accurate many-body calculation of electronic and optical band gap of bulk hexagonal boron nitride

Miroslav Kolos[1]
František Karlický[1]
[1]*University of Ostrava, Fac Sci, Dept Phys, 30 Dubna 22, CZ, 70103 Ostrava, Czech Republic*
miroslav.kolos@osu.cz

Many-body perturbational GW approximation in conjunction with the Bethe-Salpeter equation (BSE) has been employed to calculate accurate electronic and optical bandgaps of bulk hexagonal boron nitride (h-BN) in the two most important stacking configurations, AA and AB. The carefully converged results revealed h-BN as an indirect material (indirect gap approximate to 6.1 eV) with a huge excitonic effect(approximate to 0.8 eV) in perfect agreement with recent experiments [Nat.Photonics, 2016, 10, 262; Appl. Phys. Lett., 2016, 109, 122101]. The K-H region of the first Brillouin zone has been shown as the most important for the lowest optical excitations in h-BN. Surprisingly, simple scissor corrected DFT has described h-BNband structure at the GW level and subsequent time-dependent DFT with a suitable exchange-correlation kernel has provided absorption spectra similar to the fullGW+BSE spectra.