Accurate Many-body Calculation of Electronic and Optical Band Gap of Bulk Hexagonal Boron Nitride

Supplementary Information

Miroslav Kolos and František Karlický*
Department of Physics, Faculty of Science, University of Ostrava, 30. dubna 22, 701 03 Ostrava, Czech Republic

TABLE S1. Comparison of calculated direct gap (DFT and G_0W_0@DFT) and optical gap (BSE+G_0W_0@DFT) values of h-BN (AA′) using various one-particle theories. Binding energy of the first exciton, $E_b^{exc} = E_{gap,G_0W_0}^{dir} - E_{gap,BSE}^{opt}$ is added. Almost no differences in various quasiparticle gaps and in various optical gaps based on different DFT orbitals were observed, just input DFT gaps differ.

DFT	$E_{gap,DFT}^{dir}$	$E_{gap,G_0W_0}^{dir}$	$E_{gap,BSE}^{opt}$	E_b^{exc}
PBE	4.660	6.533	5.714	0.819
PBEsol	4.575	6.527	5.731	0.796
revPBE	4.728	6.588	5.715	0.873

* frantisek.karlicky@osu.cz

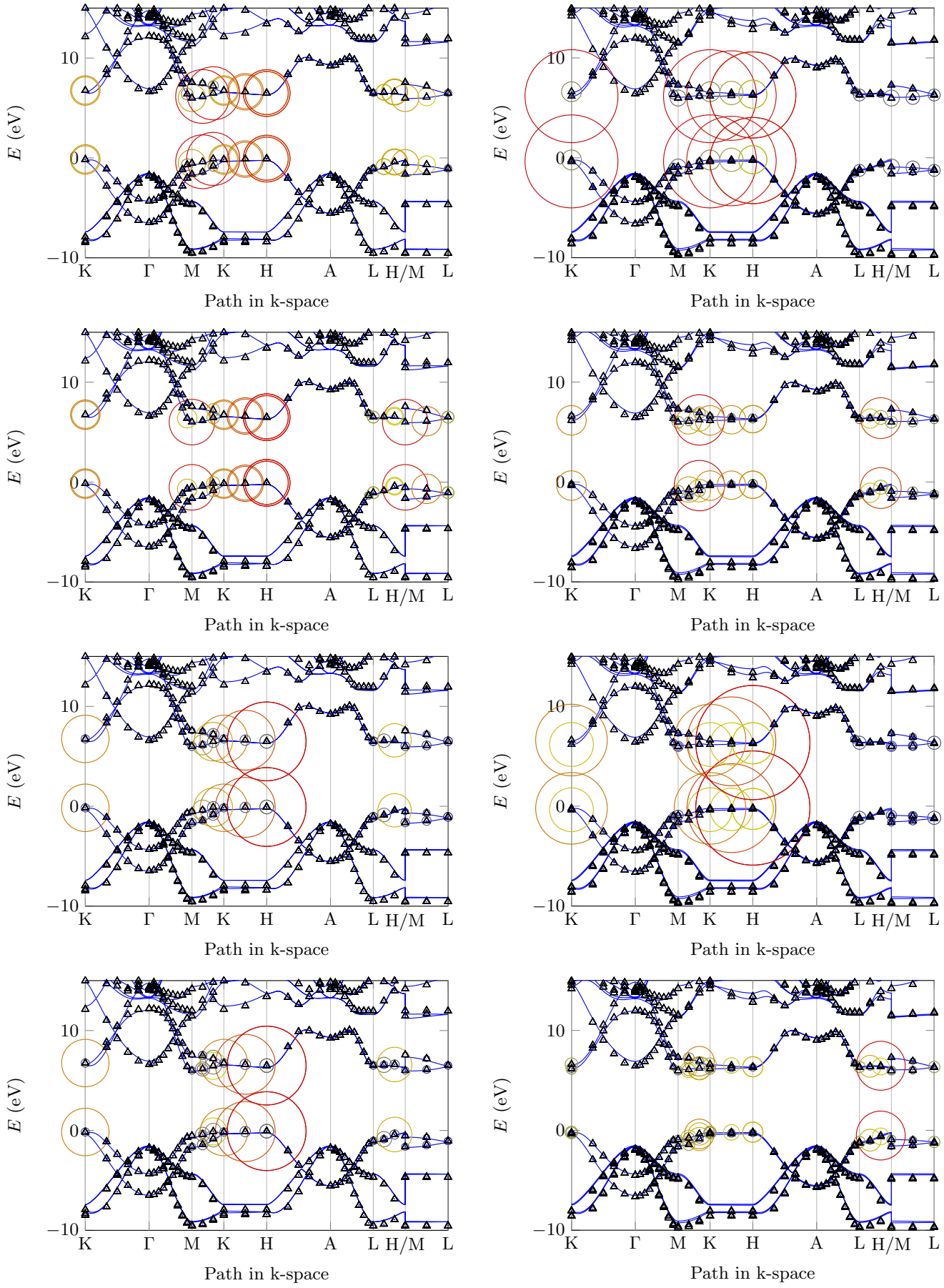

FIG. S1. Comparison of important regions in the Brillouin zone of h-BN using $A^S_{vc\boldsymbol{k}}$ coefficients (see also Eq. (1) in the main text) for first four excitations $S = 1$ (top), 2, 3, 4 (bottom). The AA′ (left) and AB (right) stacking structures of h-BN are considered and $|A^S_{vc\boldsymbol{k}}|$ (represented by radius of coloured circles; red = maximum, yellow = middle, grey = minimum) are depicted together with G_0W_0 band structure (black triangles) and PBE+Δ bands (blue lines) as a fat band structure [1].

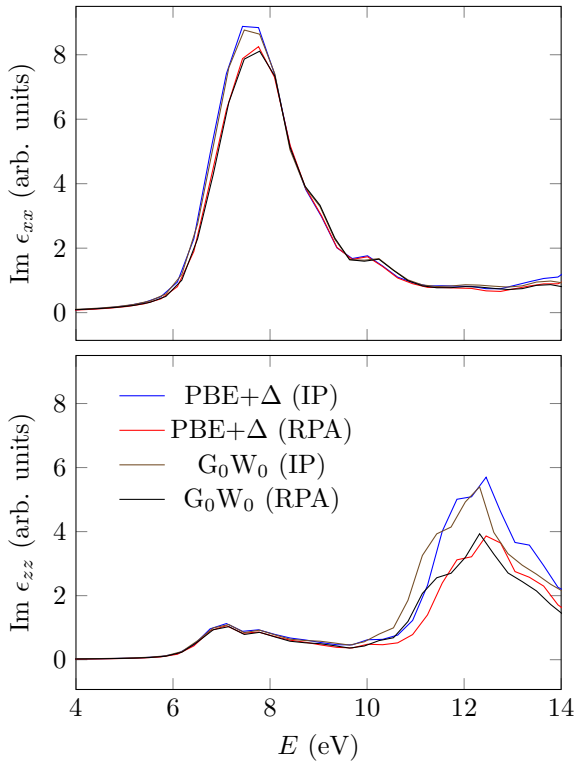

FIG. S2. Comparison of h-BN(AA′) absorption spectra (imaginary part of dielectric function ϵ) obtained from interband transitions in scissor corrected DFT (PBE+Δ) band structure and G_0W_0 band structure. Calculations with independent particle (IP) approach and with the inclusion of local field effects at random phase approximation (RPA) level are considered.

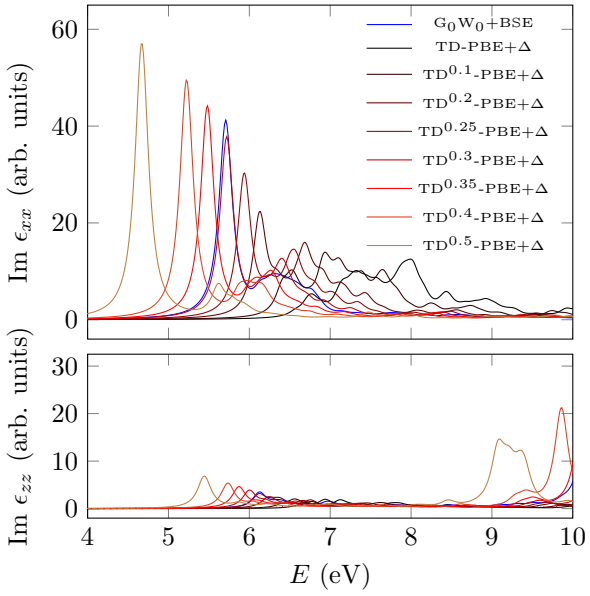

FIG. S3. Optical absorption spectra (imaginary part of dielectric function ϵ) of h-BN (AA′) using time-dependent (TD) DFT and the reference G_0W_0+BSE curve (blue line). The electron-hole ladder diagrams in present TD-DFT calculations are approximated by the exact exchange (EEX) and different EXX/GGA ratio is evaluated (and labeled by the EXX part as TD^{EXX}-PBE+Δ). We achieve surprisingly good approximation with EXX/GGA ratio of 0.3/0.7.

[1] M. Bokdam, T. Sander, A. Stroppa, S. Picozzi, D. D. Sarma, C. Franchini, and G. Kresse, Sci. Rep. **6**, 28618 (2016).