Electronic supplementary information to:

Electronic and optical properties of III-V binary 2D semiconductors: how to achieve high precision from accurate many-Body methods

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TABLE S1. Used PAW potentials recommended by VASP[1].

Element	VASP PAW type	Default cutoff (eV)	No. of explicitly treated electrons
B	B_GW	319	3
Al	Al_GW	240	3
Ga	Ga_d_GW	404	13
N	N_GW	421	5
P	P_GW	255	5
As	As_GW	209	5

TABLE S2. Technical settings for the final calculations of seven 2D materials. Super cell size for phonon calculation S_{size}, number of bands N_{bands}, GW energy cut-off E_{cut}^{GW} in eV, number of frequency grid points in GW/BSE calculation N_ω, number of k-points in band-gaps calculations N_{k-p}^{gaps}, and number of k points in spectra calculations N_{k-p}^{spec}.

Material	S_{size}	N_{bands}	E_{cut}^{GW}	N_ω	N_{k-p}^{gaps}	N_{k-p}^{spec}
BN	11×11×1	1152	200	144	18 × 18 × 1	18 × 18 × 1
BP	11×11×1	192	150	144	24 × 24 × 1	30 × 30 × 1
BAs	11×11×1	192	150	144	24 × 24 × 1	30 × 30 × 1
AlN	11×11×1	1152	200	144	18 × 18 × 1	18 × 18 × 1
GaN	9×9×1	1152	150	144	18 × 18 × 1	24 × 24 × 1
GaP	11×11×1	768	150	144	18 × 18 × 1	24 × 24 × 1
GaAs	13×13×1	768	150	144	18 × 18 × 1	24 × 24 × 1

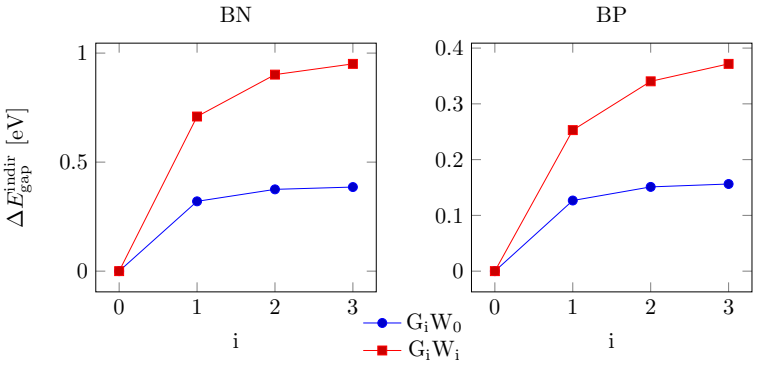

FIG. S1. Convergence of BN and BP band-gaps differences from G_0W_0 in eV with respect to number of iteration i in G_iW_0 and G_iW_i calculations.

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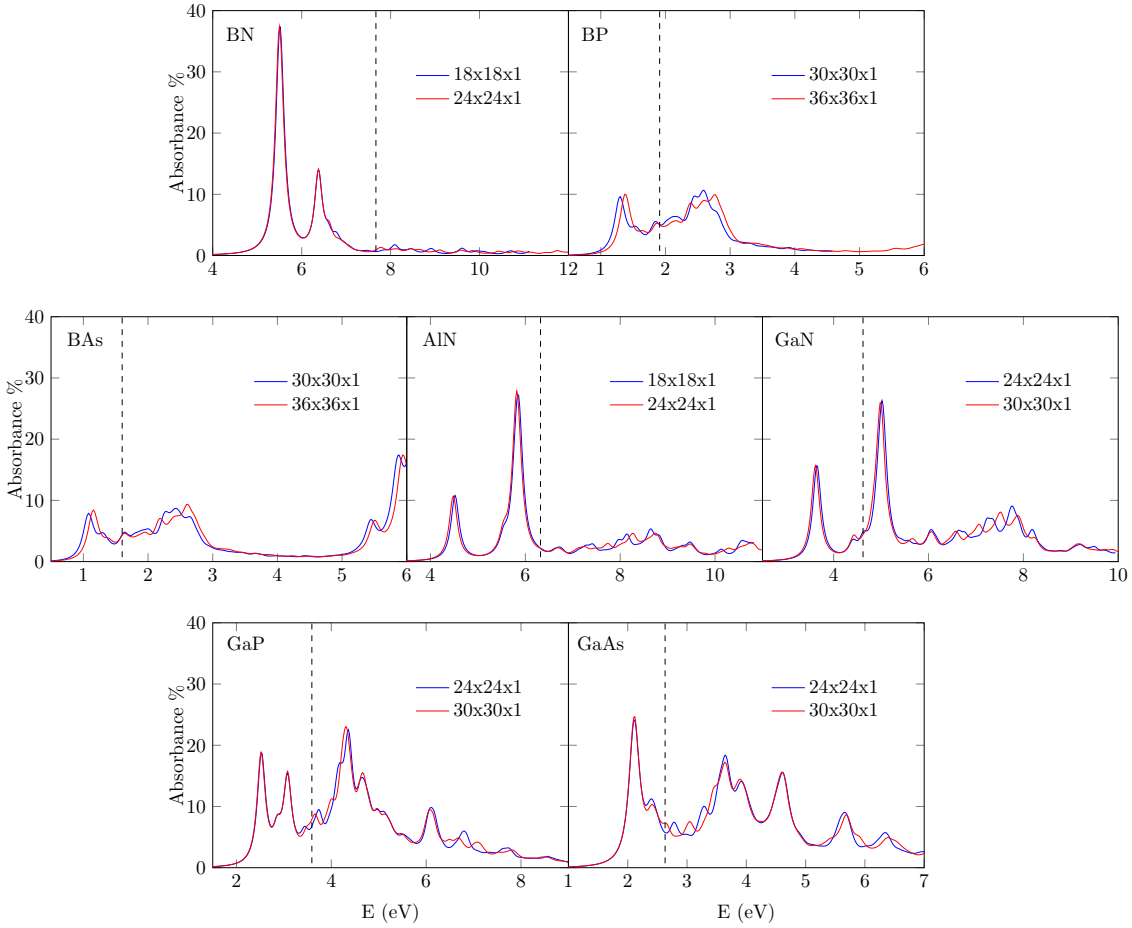

FIG. S2. Absorption spectra of seven 2D materials for different k-point sampling. Smearing width of 0.04 eV was used.

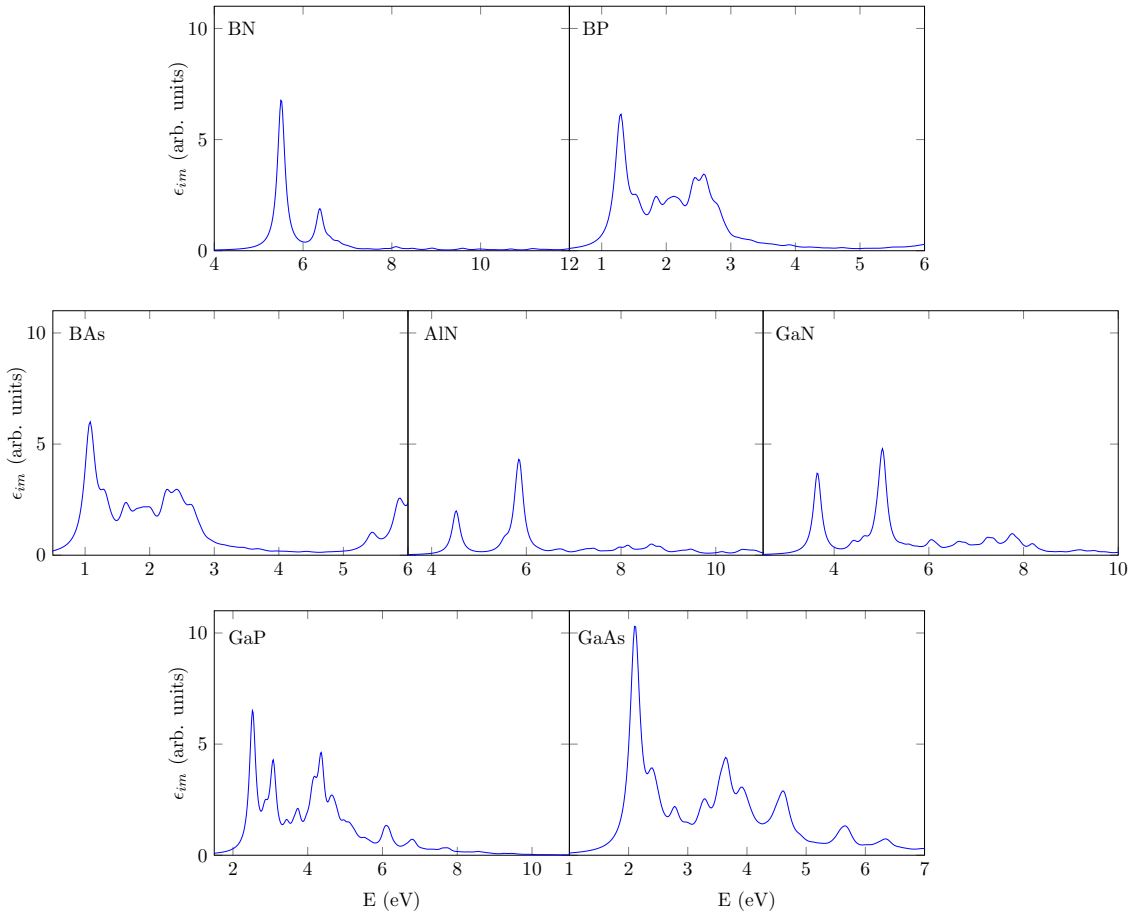

FIG. S3. Imaginary part of the dielectric function of seven 2D materials. Smearing width of 0.04 eV was used.

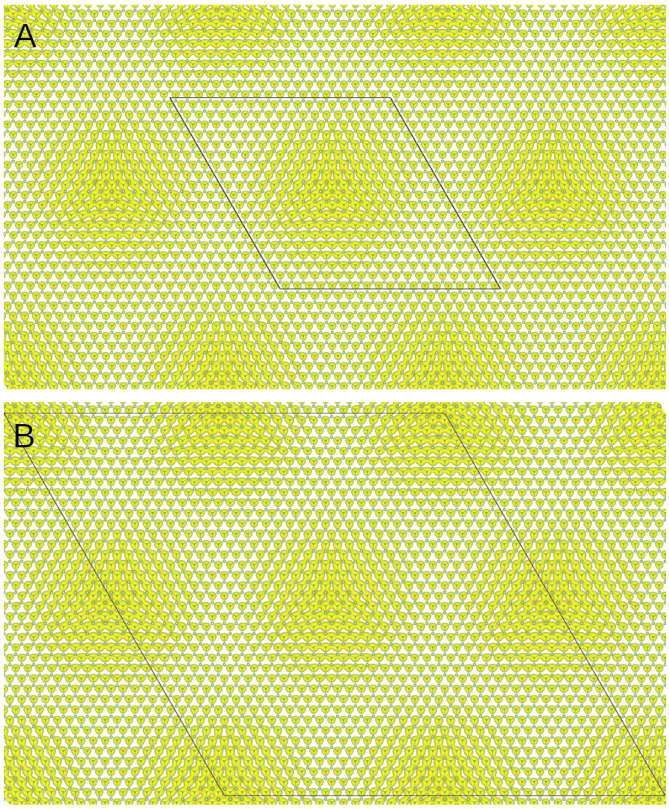

FIG. S4. Isosurface of the first bound exciton with fixed hole for BAs calculated using $18 \times 18 \times 1$ k-points. The plot uses (A) 18×18 and (B) 36×36 unit cell sizes in real space.

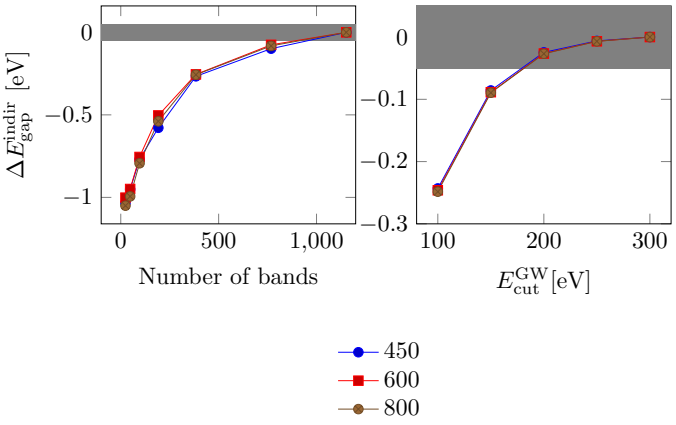

FIG. S5. Indirect gaps of BN as a function of the number of bands in the calculations and GW energy cut-off (E_{cut}^{GW}) for different plane-wave cut-offs (in legend).

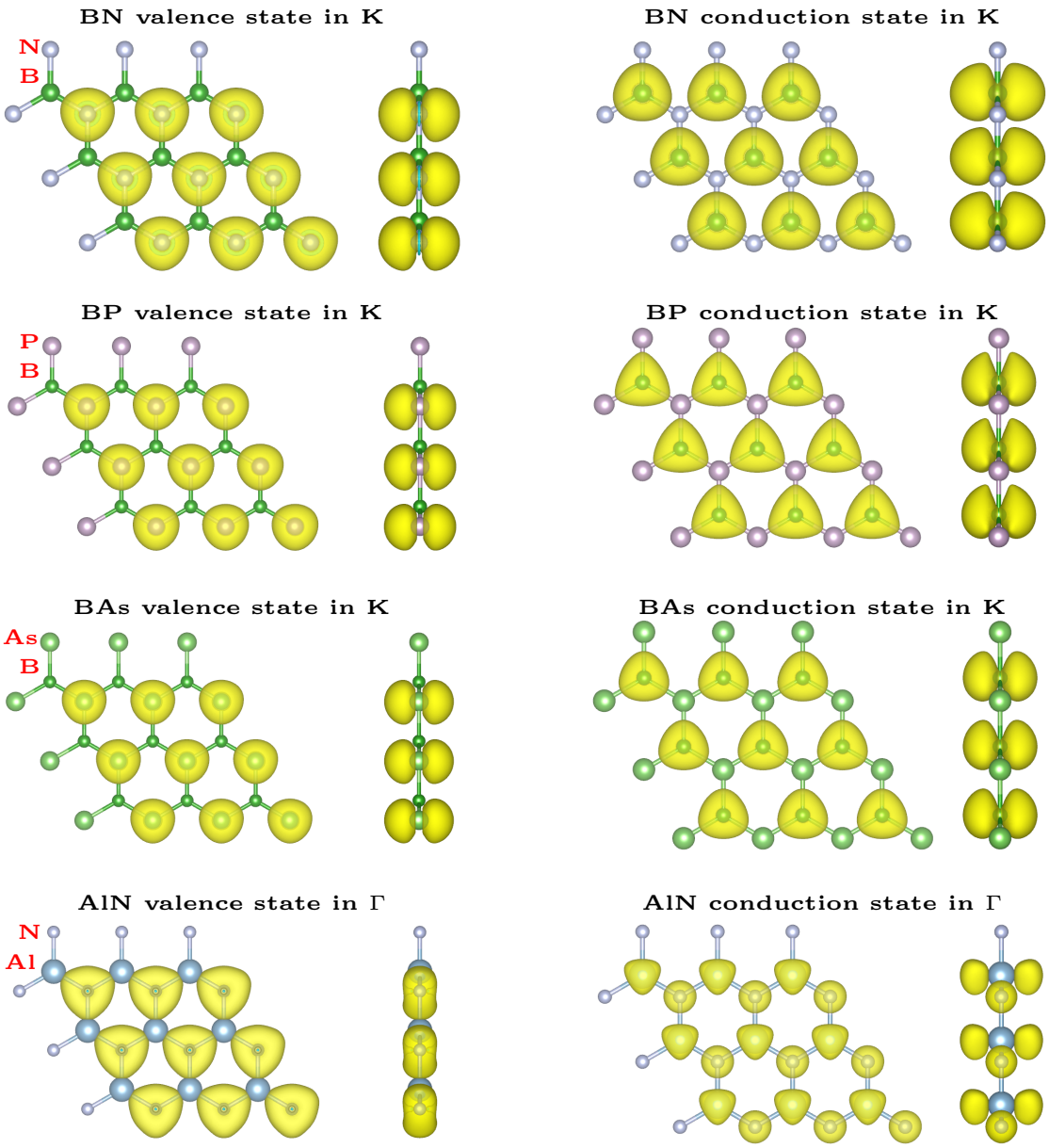

FIG. S6. Partial charges with level of 0.01 *e* corresponding to the valence and conduction bands at the k point of the direct gap location for BN, BP, BAs and AlN from PBE calculations.

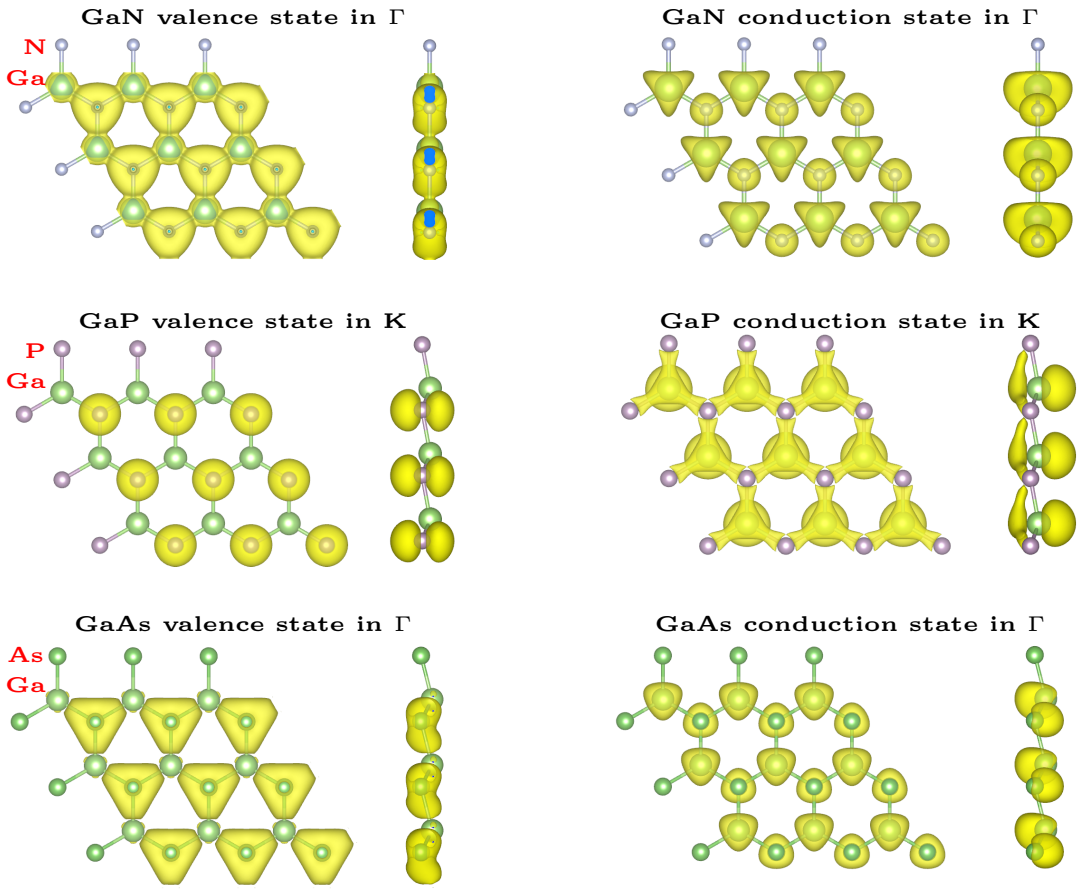

FIG. S7. Partial charges with level of 0.01 *e* corresponding to the valence and conduction bands at the k point of the direct gap location for GaN, GaP, and GaAs from PBE calculations.

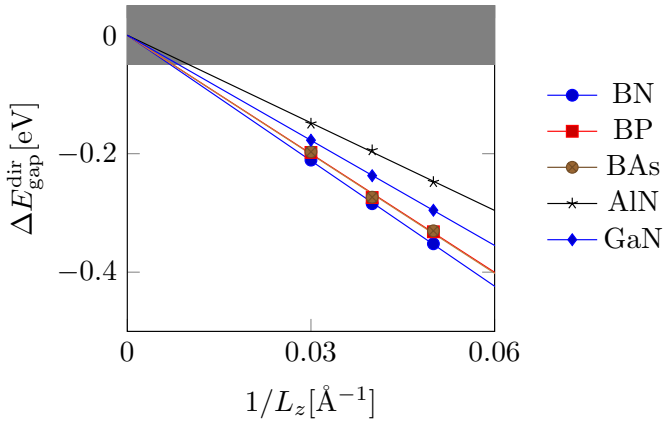

FIG. S8. Representative differences of direct G_0W_0 band-gaps ($\Delta E_{\text{gap}}^{\text{dir}}$) between converged values of five 2D materials and an extrapolated value of $\Delta E_{\text{gap}}^{\text{dir}}$ (infinite height of computational cell, $L_z \to \infty$). Grey bars show region within target ± 0.05 eV threshold.

[1] See VASP manual at https://www.vasp.at/wiki/index.php/Available_PAW_potentials.