

Stacking-dependent quasiparticle and excitonic properties of bilayer o -B₂N₂

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Orthorhombic boron nitride (o -B₂N₂) has recently emerged as a promising two-dimensional semiconductor, yet most studies have so far focused on its monolayer. Using first-principles calculations, we systematically investigate the stacking-dependent electronic structure and optical response of bilayer o -B₂N₂. We demonstrate that different stacking configurations substantially modify the electronic structure, enabling the tunability of the quasiparticle band gap between slightly below 2 and about 3 eV while preserving a direct-gap character. The optical spectra exhibit pronounced anisotropy and are dominated by strong excitonic effects in the visible region, with exciton binding energies reaching up to 0.39 eV. Analysis of the exciton wave functions reveals a stacking-driven crossover in exciton character. While the AA'', AB, and AB' stackings host tightly bound intralayer excitons, AA, AA', and AB'' favor mixed intralayer-interlayer excitons, characterized by smaller binding energies. These findings establish a direct connection between stacking configuration, quasiparticle electronic structure, and excitonic properties in bilayer o -B₂N₂, highlighting stacking engineering as an effective route for tailoring the material's optoelectronic response.

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I. INTRODUCTION

Two-dimensional materials offer remarkable opportunities for tailoring electronic, optical, and excitonic properties through structural design [1,2]. In addition to strain engineering, doping, and defect modulation, van der Waals stacking provides an especially flexible route for the tuning material properties [3,4]. Unlike three-dimensional epitaxial systems, where strict lattice matching is often required, atomically thin layers can be stacked with different interlayer registries while largely preserving the intrinsic lattice structures of the individual layers [5]. This structural freedom allows interlayer interactions to be used as an effective control parameter for emergent physical phenomena in stacked two-dimensional systems [6–9].

Orthorhombic boron nitride (o -B₂N₂) has recently attracted increasing attention as a promising two-dimensional semiconductor with potential applications in optoelectronics [10–14]. Theoretical studies have shown that monolayer o -B₂N₂ possesses an intrinsic direct band gap of approximately 1.7 eV, together with good chemical stability and strong absorption in the visible range [10,15]. These properties distinguish o -B₂N₂ from several conventional two-dimensional materials such as

graphene, silicene, and germanene, which are limited by zero or near-zero band gaps, and make it an appealing platform for exploring light-matter interactions in reduced dimensions [16]. Although o -B₂N₂ has not yet been experimentally realized, a possible synthesis route has been proposed, based on controlled reactions between suitable boron- and nitrogen-containing precursors [15]. This provides further motivation for investigating the structural and optoelectronic properties of o -B₂N₂.

Previous studies have mainly focused on the monolayer [12–14], including strain-induced modulation of its electronic, structure, and optical response, its potential applications in energy storage, and the effects of doping or defect engineering on catalytic and storage properties [10,11,17]. However, bilayers remain much less explored. This is a significant gap, because bilayer systems formed through van der Waals coupling can exhibit properties that are not simply inherited from the isolated monolayers. In fact, interlayer coupling, orbital hybridization, and stacking-dependent structural symmetry may strongly influence the electronic band structure and optical response [3,18]. In particular, different stacking configurations may exhibit direct or indirect band gaps and optical excitations, showing up in different oscillator strengths, electron-hole binding, and exciton dynamics [4,19–26]. Therefore, extending studies of o -B₂N₂ from the monolayer to bilayer systems is essential for understanding how the electronic and optical properties can be tuned by interlayer coupling.

In this work, we employ the G_0W_0 approximation [27–30] and the Bethe-Salpeter equation (BSE) [31,32] to systematically investigate the electronic structure and optical response of bilayer o -B₂N₂ in six different stacking configurations. We

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first evaluate the structural stability by analyzing the energy as a function of the interlayer distance, thereby determining their equilibrium geometries. Based on these optimized structures, we then calculate the quasiparticle (QP) band structures using the G_0W_0 method. Finally, by solving the BSE, we explicitly include electron-hole interactions and analyze how the stacking configuration influences the optical absorption spectra, including excitonic features. This study establishes a clear stacking-property relationship on a theoretical basis and provides useful guidelines for optimizing the stacking configuration of α -B₂N₂ [33–35].

II. COMPUTATIONAL DETAILS

Structure optimizations were performed using the all-electron code FHI-aims [36]. Long-range dispersion interactions were included through the many-body dispersion van der Waals method (vdW-MBD) [37,38]. Thereby, the in-plane lattice constants were fixed at the monolayer values of $a = 4.57$ Å and $b = 2.50$ Å as obtained with the Perdew-Burke-Ernzerhof (PBE) functional. For each stacking configuration, the atomic positions were relaxed to determine the equilibrium interlayer distance, until the residual interatomic forces were below 10^{-3} eV Å⁻¹. A vacuum spacing of 15 Å was used, and a Coulomb cutoff was applied

in order to eliminate spurious interactions between periodically repeated slabs in out-of-plane direction. All subsequent ground-state, G_0W_0 , and BSE calculations are performed using exciting [39,40], an all-electron full-potential code, implementing the family of linearized augmented plane wave plus local orbitals (LAPW + LO) methods. For both atomic species involved, namely boron (B) and nitrogen (N), a muffin-tin radius $R_{MT} = 1.3$ bohrs is adopted and a basis-set cutoff of $R_{MT}G_{max} = 7$ is used. The sampling of the Brillouin zone (BZ) is carried out with an $8 \times 14 \times 1$ k grid. Calculations of the QP corrections to the Kohn-Sham eigenvalues are performed within the G_0W_0 approximation using 400 empty states and a shifted $6 \times 10 \times 1$ k -point mesh. A two-dimensional (2D) cutoff of the bare Coulomb potential and a special treatment of the $\mathbf{q} = \mathbf{0}$ term are applied in the G_0W_0 calculations [41–43]. Convergence tests with respect to the relevant numerical parameters indicate that the QP gap at the high-symmetry point Γ is converged within about 70 meV. High-resolution G_0W_0 QP band structures are obtained by Wannier interpolation [44]. The optical spectra are calculated by solving the BSE [45] with the same treatment of the 2D Coulomb cutoff and the $\mathbf{q} = \mathbf{0}$ singularity as in the G_0W_0 calculations. A plane-wave cutoff of $R_{MT}G_{max} = 6$ is employed. The response function and the screened Coulomb potential are calculated including 100 empty bands. The BSE

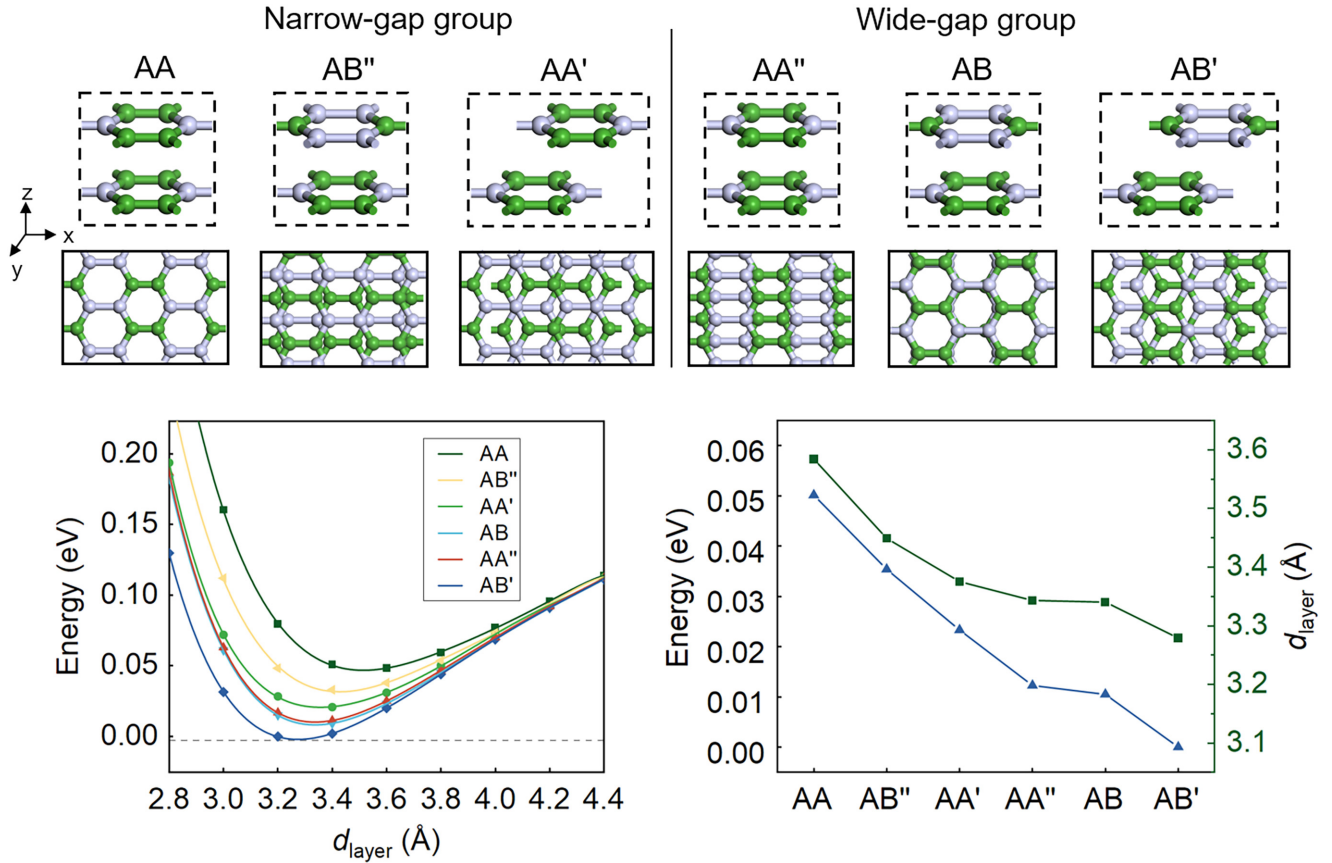


FIG. 1. Side and top views of the six investigated stacking configurations AA, AB'', AA', AA'', AB, and AB' of bilayer α -B₂N₂. Bottom left: Total energy of these configurations as a function of the interlayer distance d_{int} , with the minimum energy of the AB' configuration taken as the reference. Bottom right: Relative energies of the different stacking configurations at their equilibrium interlayer distances, which are shown on the right axis.

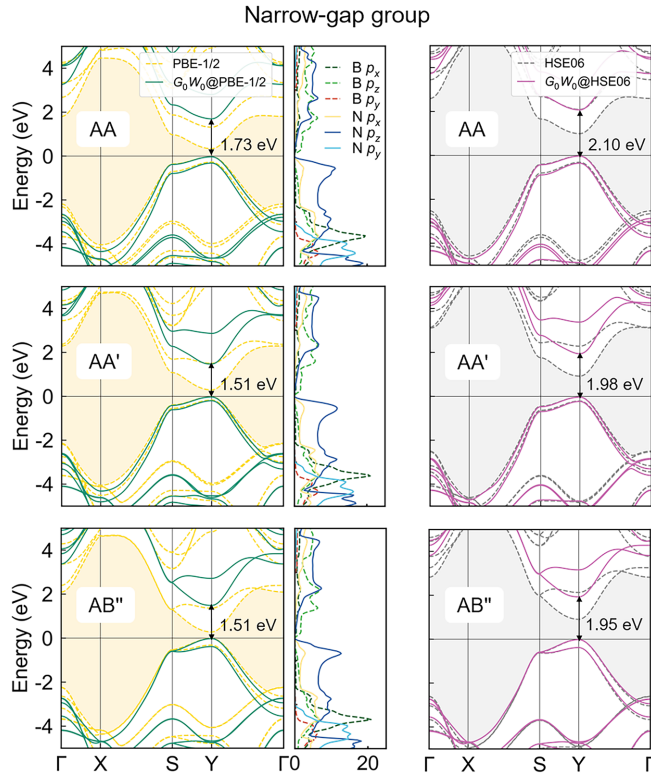


FIG. 2. Electronic band structures and projected densities of states (DOS) for the narrow-gap configurations AA, AA', and AB''. The left panels show the PBE-1/2 and G_0W_0 @PBE-1/2 band structures, together with the atom- and orbital-projected DOS resolved from PBE-1/2. The right panels show the corresponding results from HSE06 and G_0W_0 @HSE06. The valence-band maximum is set to zero in all panels, and the arrows indicate the quasiparticle gaps.

Hamiltonians are constructed using six occupied and six unoccupied bands and a $16 \times 28 \times 1$ k -point mesh shifted by (0.01, 0.015, 0.05) expressed in fractional reciprocal-lattice coordinates. Shifted meshes have been shown to improve the BZ sampling and thus the convergence of optical spectra [1]. These parameters yield well-converged spectra, and the energy of the first exciton is converged within about 10 meV. A Lorentzian broadening of 0.1 eV is applied to the resulting spectra.

TABLE I. Band gaps of monolayer and bilayer α -B₂N₂ obtained by PBE, PBE-1/2, HSE06, GW@PBE, GW@PBE-1/2, and GW@HSE together with the interlayer distance d_{int} obtained by vdW-corrected PBE.

System	d_{int} (Å)	Band gap (eV)					
		PBE	PBE-1/2	HSE06	GW@PBE	GW@PBE-1/2	GW@HSE
Monolayer		0.64	0.98	1.71	2.24	2.84	3.17
Monolayer [15]		0.64		1.70			
AA	3.58	0.00	0.37	1.02		1.73	2.10
AA'	3.38	0.00	0.32	0.96		1.51	1.98
AB''	3.45	0.00	0.30	0.93		1.51	1.95
AA''	3.34	0.67	0.98	1.72	1.92	2.47	2.86
AB	3.34	0.69	1.02	1.76	1.99	2.55	2.92
AB'	3.28	0.69	1.00	1.73	1.95	2.49	2.87

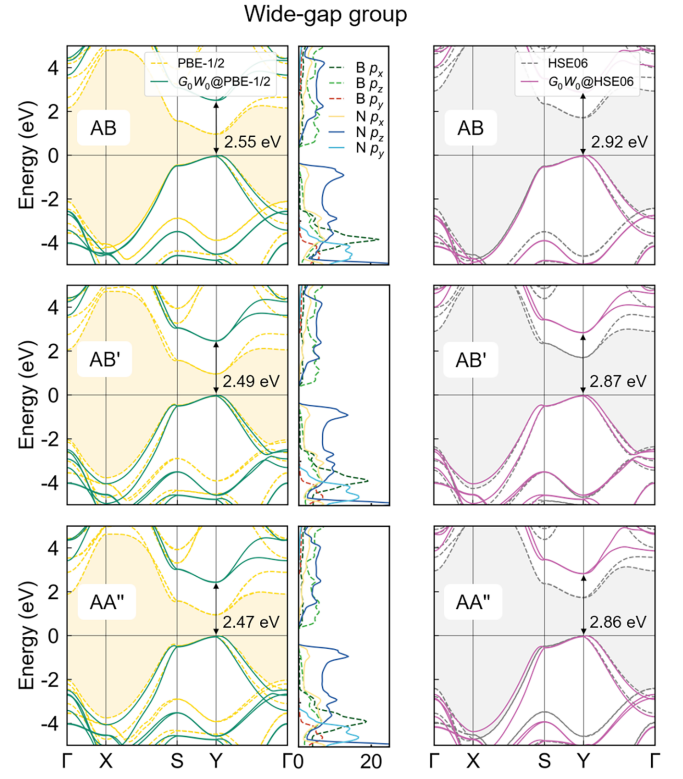


FIG. 3. Same as Fig. 2 but for the wide-gap configurations AB, AB', and AA''.

III. RESULTS AND DISCUSSION

A. Structural properties

To clarify how the stacking configuration affects the structural properties of bilayer α -B₂N₂, we first analyze the relative stability of the six investigated systems as a function of interlayer distance. Taking the lowest-energy configuration AB' as the reference, the relative stability and the equilibrium interlayer distance are shown in the bottom panels of Fig. 1. For each stacking configuration, the total-energy curve as a function of interlayer distance exhibits a clear minimum, confirming the existence of a stable equilibrium spacing between the two layers. The resulting interlayer distances range from 3.28 to 3.58 Å, as shown in Table I. The AA, AA', and AB'' configurations display markedly higher energies, which

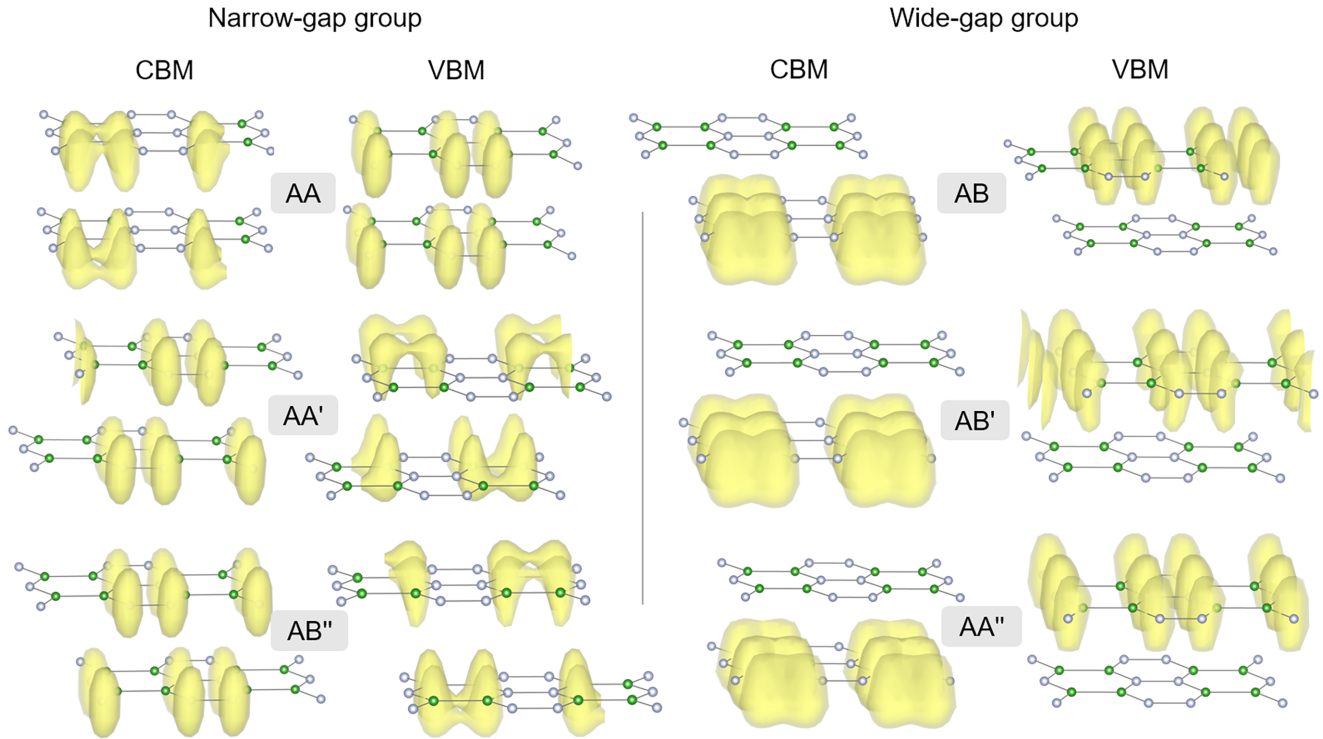


FIG. 4. Real-space distributions of the CBM and VBM Kohn-Sham states obtained from PBE-1/2. The yellow isosurfaces represent $|\psi|^2$ plotted at an isovalue of 6×10^{-5} .

can be primarily attributed to strong electrostatic repulsion arising from the vertical alignment of identical atomic species, thereby increasing the interlayer separation. In contrast, in the AA'', AB and AB' configurations, B (N) atoms preferentially align with N (B) atoms in the adjacent layer or with the centers of the hexagons, effectively reducing interlayer repulsion and rendering the systems energetically more stable. Overall, the lowest-energy configuration corresponds to the smallest equilibrium interlayer distance. The dynamical stability of all six stacking configurations is evidenced by computing their phonon dispersions within the harmonic approximation, which do not show any imaginary frequencies.

B. Electronic structure

Before investigating the effects of stacking on the electronic structure, we first calculate monolayer o -B₂N₂ as a reference. The electronic structure and the optical spectrum agree well with previous reports [10,15] and are summarized in the Appendix (Fig. 7). The band gaps of the six stacking configurations obtained at different levels of theory are summarized in Table I. At the PBE level, the electronic character is found to be highly sensitive to the stacking. The AB, AB', and AA'' configurations are semiconducting, with direct band gaps of 0.67–0.69 eV at the Γ point, whereas the AA, AA', and AB'' configurations exhibit vanishing band gaps, indicating semimetallic behavior obtained by semilocal DFT. Such a gap closure at the PBE level poses a challenge for subsequent G_0W_0 calculations, because a strongly underestimated gap at the starting point can lead to an overestimated polarizability and hence to an overscreened Coulomb interaction [46].

To avoid this problem, we employ PBE-1/2 as the starting point for the QP calculations for all systems [47]. In this method [48], an approximate self-energy correction is introduced exploiting the idea of Slater's transition state. The correction potential is constructed from the difference between the potentials of a neutral and a half-ionized atom and is added to the Kohn-Sham potential, trimmed by a cutoff radius. For practical reasons, we apply here the PBE-1/2 correction as a scissors operator to rigidly shift the conduction bands, in a spirit similar to DFT + U, rather than following its original self-energy concept. This provides a computationally efficient means of enlarging band gaps while retaining a PBE-like computational cost. To avoid double counting in the subsequent G_0W_0 calculations, the PBE-1/2 contribution to the band-gap correction is accordingly subtracted when evaluating the QP corrections [47,49]. A similar strategy has also been adopted in previous studies [47,48,50,51]. Figure 2 shows the electronic band structures of the narrow-gap configurations AA, AA', and AB''. The left panels present the PBE-1/2 band structures and the corresponding G_0W_0 results based on PBE-1/2 ($G_0W_0@PBE-1/2$), while the right panels show the HSE06 band structures and the corresponding G_0W_0 results based on HSE06 ($G_0W_0@HSE06$). At the PBE-1/2 level, the calculated gaps of these three configurations are 0.30–0.37 eV. Upon applying the G_0W_0 self-energy corrections, the quasiparticle gaps increase to 1.51–1.73 eV. At the HSE06 level, larger gaps of 0.93–1.02 eV are obtained, and the corresponding $G_0W_0@HSE06$ quasiparticle gaps further increase to 1.95–2.10 eV. Although the absolute gap values depend on the chosen starting point, the relative trend among these configurations is consistently preserved.

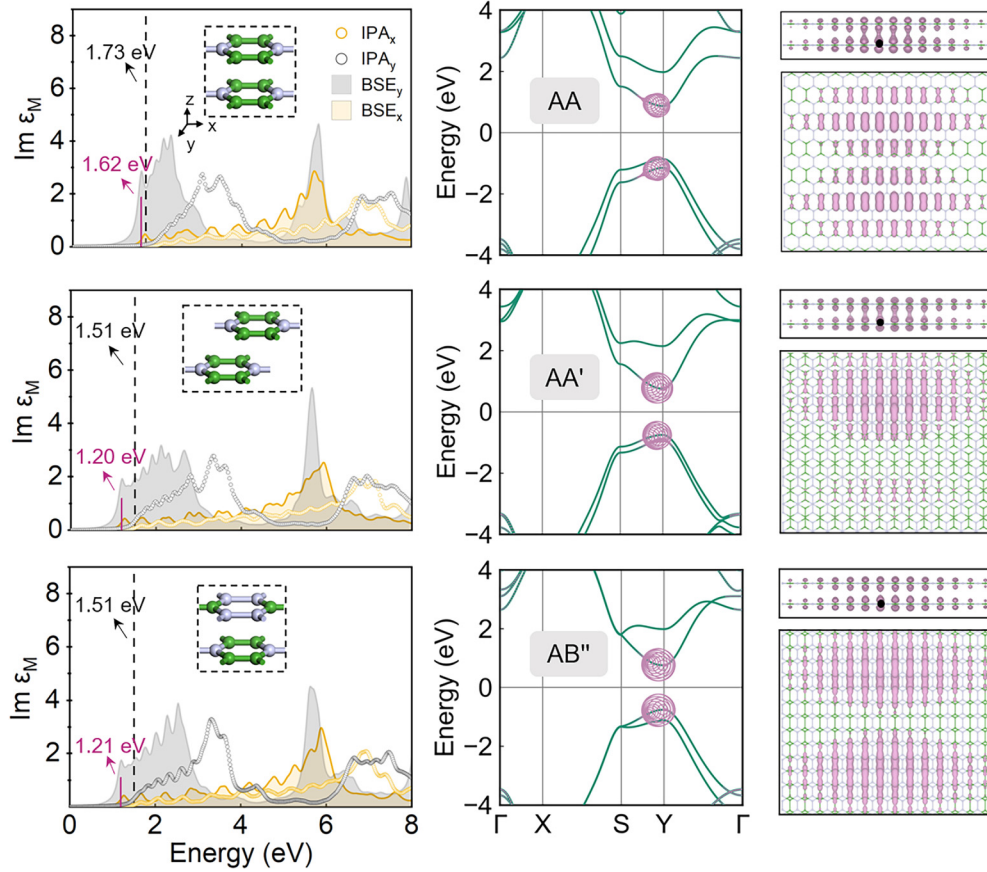


FIG. 5. Optical properties of bilayer o -B₂N₂ for the stacking configurations AA, AA', and AB'' (from top to bottom). The left panels show the in-plane components of the imaginary part of the macroscopic dielectric tensor, obtained from the Bethe-Salpeter equation (colored areas). For comparison, the results from the independent-particle approximation (IPA) are shown (dashed lines). A Lorentzian broadening of 0.1 eV is applied to all spectra. The first bright exciton is highlighted by the pink vertical line. The dashed lines indicate the respective direct QP gaps. The middle panels depict the reciprocal-space distribution of the corresponding first bright exciton. The size of the pink circles represents the band contribution at the k points involved in the excitation. The right panels show the real-space distributions of the electron (side and top views) for fixed hole coordinate (black dot), represented by the pink isosurfaces. B atoms are shown in green and N atoms in grey.

Figure 3 presents the corresponding results for the wide-gap configurations AB, AB', and AA''. At the PBE-1/2 level, these stackings show larger gaps of 0.98–1.02 eV. The G_0W_0 @PBE-1/2 quasiparticle gaps are 2.47–2.55 eV. HSE06 gives the same overall trend, with gaps of 1.72–1.76 eV that increase to 2.86–2.92 eV at the G_0W_0 @HSE06 level. Thus the relative variation among these stacking configurations is also reproduced when using HSE06 as the starting point.

Overall, the comparison between Figs. 2 and 3 shows that the absolute band gaps are starting-point dependent, as expected. Nevertheless, the stacking-dependent variation and the relative ordering of the band gaps are consistently maintained at both the PBE-1/2/ G_0W_0 @PBE-1/2 and HSE06/ G_0W_0 @HSE06 levels. This confirms that the pronounced dependence of the electronic structure of bilayer o -B₂N₂ on the stacking configuration is robust with respect to the choice of starting point.

To get further insight into the origin of the stacking dependence of the band gap, we analyze the orbital contributions and real-space distributions of the band-edge states. As is evident from the projected density of states (PDOS) in Figs. 2 and 3, both the valence-band maximum (VBM) and the

conduction-band minimum (CBM) are mainly derived from the p orbitals of B and N atoms, with the out-of-plane p_z orbitals dominating near the band edges. This explains sensitivity of the band-edge states to the relative atomic registry between the two layers, which result in differences in the QP gap by about 1 eV.

The real-space distributions of the CBM and VBM provide a more direct picture of how the band-edge states respond to different stacking configurations. Figure 4 compares the corresponding Kohn-Sham states of all six stackings. In the narrow-gap group, AA, AA', and AB'', the band-edge states are generally distributed over both layers, indicating pronounced interlayer hybridization. In this group of stackings, atoms in the upper and lower layers are nearly vertically aligned, and both the CBM and VBM exhibit pronounced out-of-plane distributions extending across the two layers. In contrast, in the wide-gap group, AB, AB', and AA'', the band-edge states exhibit more layer-selective distributions, reflecting reduced interlayer overlap. The different atomic registry between the two layers leads to a more asymmetric distribution of the band-edge states, with the CBM mainly localized in one layer and the VBM in the other.

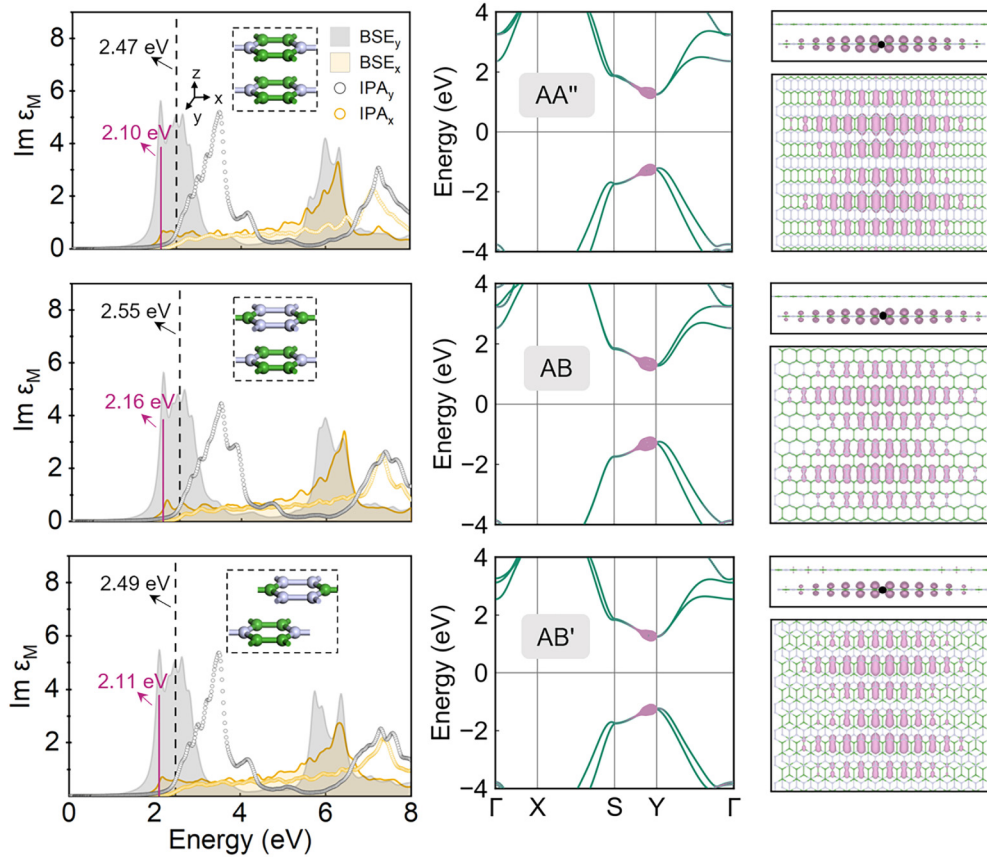


FIG. 6. Same as Fig. 5, but for the stacking configurations AA'', AB, and AB'.

These stacking-induced changes in the spatial character of the band-edge states can modify their relative energies, thereby contributing to the large variation of the quasiparticle band gap in bilayer $o\text{-B}_2\text{N}_2$. This highlights the important role of interlayer atomic registry in tuning the electronic structure of bilayer $o\text{-B}_2\text{N}_2$.

C. Optical properties

Given that dielectric screening is substantially weakened in two-dimensional van der Waals systems compared to bulk materials, electron-hole interactions are strongly enhanced, thus excitonic effects characterize their optical response. On the basis of the QP band structures, we use the BSE to systematically investigate the optical absorption of the considered materials. We first discuss the three configurations with the smaller gaps, namely AA, AA', and AB''. As shown in Fig. 5, the absorption spectra of these configurations undergo a pronounced reconstruction compared with the independent-quasiparticle (IPA) results. They exhibit clear in-plane anisotropy. Along the y direction, the lowest-energy absorption peaks are located at 1.62 eV for AA and at nearly identical energies of 1.20 and 1.21 eV for AA' and AB'', respectively. Compared with the corresponding QP band gaps of 1.73, 1.51, and 1.51 eV, these peaks yield exciton binding energies of 0.11, 0.31, and 0.30 eV. The absorption along the x direction is much weaker in the low-energy region, highlighting the pronounced in-plane anisotropy of the optical response. To clarify the transitions establishing the

excitonic states, we analyze the contributions in reciprocal space. As shown in the middle column of Fig. 5, in all three materials, the exciton weight is mainly concentrated around the Y point, indicating that the lowest-energy bright exciton primarily originate from multiple electron-hole transitions near the band edges, while transitions at the fundamental gap are forbidden, since CBM and VBM are both of p character.

For visualizing the spatial characteristics of the excitonic states, we plot the real-space distributions of the squared exciton wavefunction in the right column of Fig. 5. In these calculations, the hole is fixed at the position of an N atom, since the valence-band-edge states are dominated by the p_z orbitals of nitrogen atoms. In all cases, the spatial distribution is rather extended, with the lateral size of the wavefunctions covering about 14 unit cells. Notably, the excitons are distributed over both the upper and lower layer, with very similar density and extension, indicating their intralayer character. This partial spatial separation of the electron and hole effectively weakens the Coulomb interaction, thereby leading to a relatively small exciton binding energies.

We provide a similar analysis for the AA'', AB, and AB' stacking configurations in Fig. 6. These three stackings exhibit stronger absorption intensities in the low-energy region, and their lowest bright exciton peaks appear at slightly higher energies. The lowest bright exciton peaks are located at 2.10, 2.16, and 2.11 eV, respectively, with exciton binding energies of 0.37–0.39 eV, which are slightly larger than those of the narrow-gap configurations. The middle column of Fig. 6

shows the corresponding exciton weights in reciprocal space. As in the other cases, they are mainly concentrated near the band-edge region around the Y point. Although the overall distribution patterns are similar to those, there are small differences in the spatial extent and intensity of the exciton weights, reflecting a certain sensitivity of the excitonic states to the stacking configuration. The corresponding real-space distributions of the squared exciton wave functions are shown in the right panels of Fig. 6. In all three cases, they exhibit relatively localized and nearly symmetric in-plane distributions, indicative of the larger binding energies. In all three cases, the excitons are localized in one layer.

Overall, these results show that stacking affects not only the quasiparticle band gaps, but also the optical absorption spectra, also in terms of binding energies and real-space distributions of the lowest bright excitons. This indicates that the nature of the exciton wave functions can be tuned by the stacking-controlled atomic registry: AA'' , AB , and AB' tend to form predominantly intralayer excitons at the absorption onset, whereas those of AA , AA' , and AB'' exhibit a more pronounced mixed intralayer/interlayer character.

IV. SUMMARY AND CONCLUSIONS

In summary, using many-body perturbation theory, we have systematically investigated the stacking-dependent

quasiparticle and excitonic properties of bilayer orthorhombic boron nitride (o - B_2N_2). The G_0W_0 calculations show that all bilayer systems retain a direct band-gap character, however, the QP band gap is highly sensitive to the stacking configuration, with gap variations of about 1 eV. Solving the BSE based on the QP band structures demonstrates that bilayer o - B_2N_2 exhibits pronounced excitonic effects and optical anisotropy in the visible region. In the AA'' , AB , and AB' stackings, the first bright exciton exhibits relatively large binding energies of about 0.37–0.39 eV. In contrast, in the AA , AA' , and AB'' stackings, the corresponding binding energies are only 0.11–0.31 eV. A real-space analysis of the exciton wave functions reveals two intrinsically different types of excitonic states: In AA'' , AB , and AB' configurations, excitons are mainly localized within a single layer, manifesting as strongly bound intralayer excitons. In contrast, in AA , AA' , and AB'' configurations, the enhanced interlayer coupling leads to exciton wave functions distributed across both layers. These mixed excitonic states with coexisting intralayer and interlayer character explains their relatively small exciton binding energies. Overall, van der Waals bilayer o - B_2N_2 not only exhibits enhanced tunability in terms of structural and QP band properties but also in its exciton response, offering a flexible platform for controllable exciton engineering. These results establish a solid theoretical foundation for considering this material for optoelectronic applications.

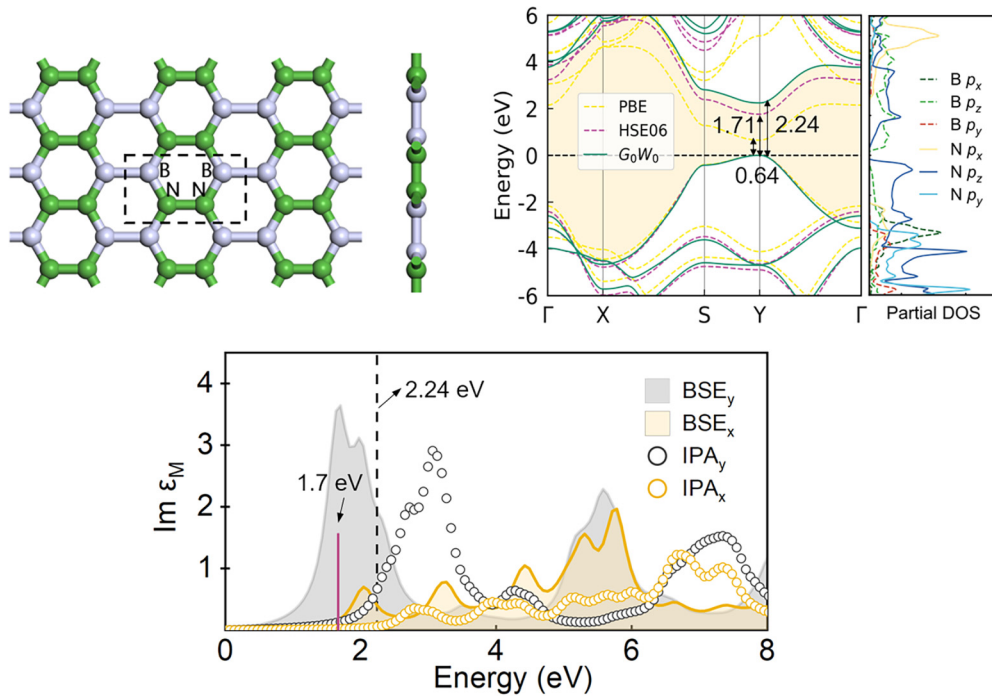


FIG. 7. Structural, electronic, and optical properties of monolayer o - B_2N_2 . Top left: Top and side view of the relaxed structure. The dashed rectangle indicates the primitive cell. Top right: Electronic band structures obtained with PBE, HSE06, and G_0W_0 @PBE, together with the orbital-projected density of states. The valence-band maximum is set to zero, and the arrows indicate the respective band gaps. Bottom: Imaginary part of the macroscopic dielectric function calculated within the independent-particle approximation (IPA) and the Bethe-Salpeter equation (BSE) for light polarized along the x and y directions. The dashed vertical line marks the direct G_0W_0 gap.

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DATA AVAILABILITY

Input and output files of all calculations can be downloaded free of charge from the NOMAD data infrastructure [53] by the following Ref. [54].

APPENDIX: MONOLAYER o -B₂N₂

The reference results for monolayer o -B₂N₂ are shown in Fig. 7.

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