Supporting Information (SI)
for

Excitonic circular dichroism in boron-nitrogen clusters decorated graphene

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A. Cohesive Energy Calculation

Employing the cohesive energy calculation, we verify the stability and potential experimental realization of the BNcG system, using the following expression:

$$E_{cohesive} = E_{BNcG} - 24\,E_C - 3\,E_N - 3\,E_B - E_{hBN}$$

here E_{BNcG}, E_{hBN}, E_C, E_N, and E_B are the total energies of the BNcG system, hBN system, and the energies of carbon (C), nitrogen (N), and boron (B) atoms in their sp^2 hybridized planar structures, respectively. The term E_C is calculated by considering half of the energy of a two-atom graphene unit cell (E_{CC}). E_{hBN} denotes the ground state energy of the two-atom unit cell consisting of one B and one N atom. The BNcG unit cell consists of 3 nitrogen and 3 boron atoms, which are connected to the carbon atoms. To replicate these sp^2 hybridized environments, E_N and E_B are calculated from the two-dimensional monolayer honeycomb lattices, C_3N and BC_3, respectively from their 8-atom unit cells as per the following expressions:

$$E_B = (E_{BC3} - 3E_{CC})/2$$

$$E_N = (E_{C3N} - 3E_{CC})/2$$

As per our calculations,

E_{BNcG} = -285.235 eV

E_{CC} = -18.4711 eV

E_{hBN} = -17.5967 eV

E_{BC3} = -67.227 eV

E_{C3N} = -70.33 eV

From the above expressions, we derive the following energies for single atoms,

E_C = -9.235 eV

E_N = -7.458 eV

E_B = -5.907 eV

Incorporating all the above energy values, we finally obtain the cohesive energy, $E_{cohesive}$ = -5.9 eV for the total BNcG unit cell consisting of a total of 50 atoms. Therefore, the cohesive energy per atom comes out to be -184.4 meV. This negative cohesive energy indicates the stability of the BNcG system.

B. Convergence test of GW calculations

We first consider the total number of bands including the valance and conduction band to calculate the dielectric matrix with a **k**-point mesh of 10 x 10 x 1, dielectric matrix cut-off of 10 Ry, and bare Coulomb cut-off 60 Ry as shown in Table S1. Then fixing the number of bands at 702 and by varying the dielectric matrix cut-off we achieve the convergence in the dielectric matrix with a 10 x 10 x 1 as shown in Table S1. Following this, with the fixed dielectric cut-off at 10 Ry, 702 bands, and 10 x 10 x 1 **k**-point we test the convergence on the bare Coulomb cut-off as shown in Table S2. We find 100 Ry the converged bare Coulomb cut-off. Finally, we assess the convergence for the coarse **k**-grid and find that 10 x10 x 1 as a converged **k**-grid as shown in Table S1.

Table S1: N_b is the number of bands (occupied plus unoccupied), E_g in (eV) is the *GW* gap, Encut (in Ry) is the energy cut-off of the plane wave, Epsilon-cut (in Ry) is the dielectric matrix cut-off in the epsilon calculations.

N_b	E_g	Epsilon-cut	E_g	Encut	E_g	**k**-point	E_g
502	2.30	8	2.29	40	2.29	8 x 8 x 1	2.28
602	2.29	9	2.29	50	2.29	9 x 9 x 1	2.31
702	2.29	10	2.29	60	2.29	10 x 10 x 1	2.29

C. Convergence test of BSE calculations

To achieve the convergence of Bethe-Salpeter equation (BSE), we vary the number of valance and conduction bands. We find 3 valence bands and 4 conduction bands are the converged parameters in the BSE calculation. Then we test convergence by varying the **k**-grid in BSE calculations. We find 24 x 24 x 1 is the converged **k**-grid. The absorption plot of the singlet exciton of the BNcG system is shown in FIG. S1.

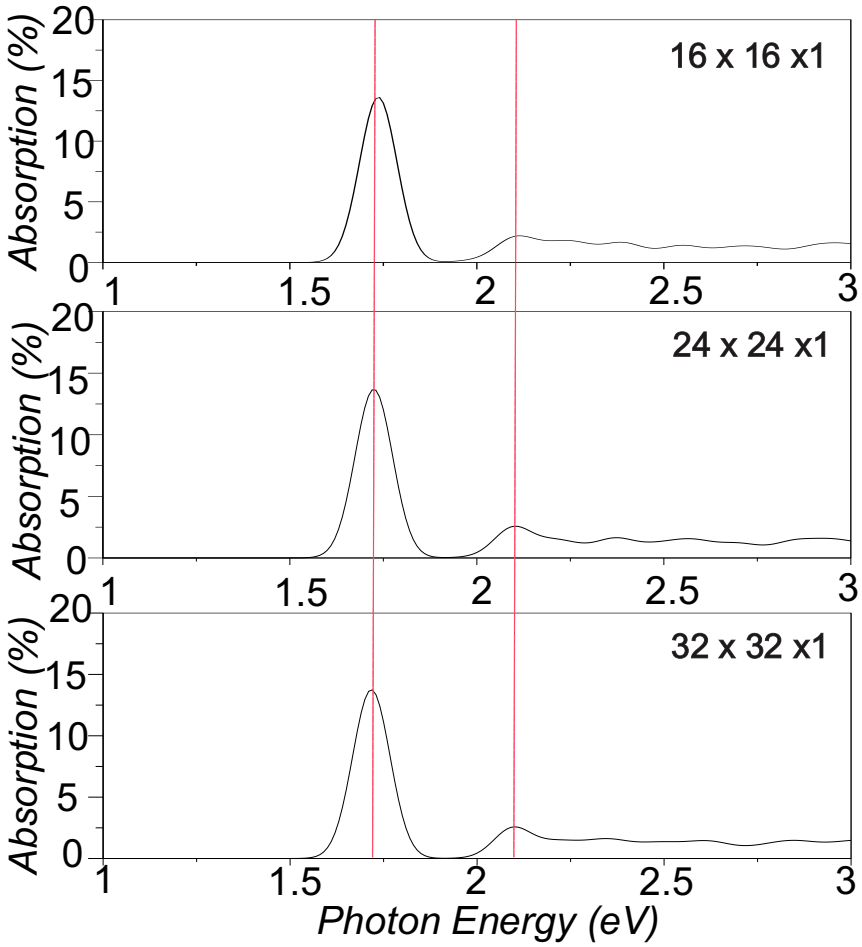

FIG. S1: BSE convergence test with 3 valence bands and 4 conduction bands. The top, middle, and bottom panels represent the absorption spectra of BNcG obtained from **k**-grids of 16 x 16 x 1, 24 x 24 x 1 and 32 x 32 x 1, respectively.

D. Original plots of Fig. 4 in the main text

The original plots of Fig.4 in the main text are provided here. Using a Python code given in the GitHub repository (bgwtools) of the BerkeleyGW package we obtain these plots. For improved visualization, we rotated all figures by a 45° angle, ensuring that the first Brillouin zone appears as a perfect hexagon, as depicted in Fig. 4 of the main text.

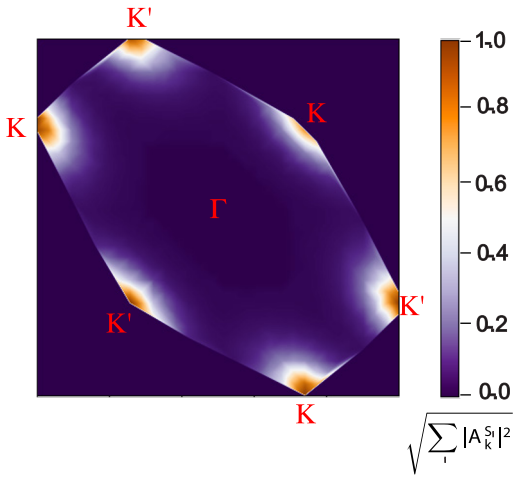

FIG. S2: The square root of the sum of the squared excitonic envelope function of the first bright singlet exciton of BNcG over the hexagonal first BZ.

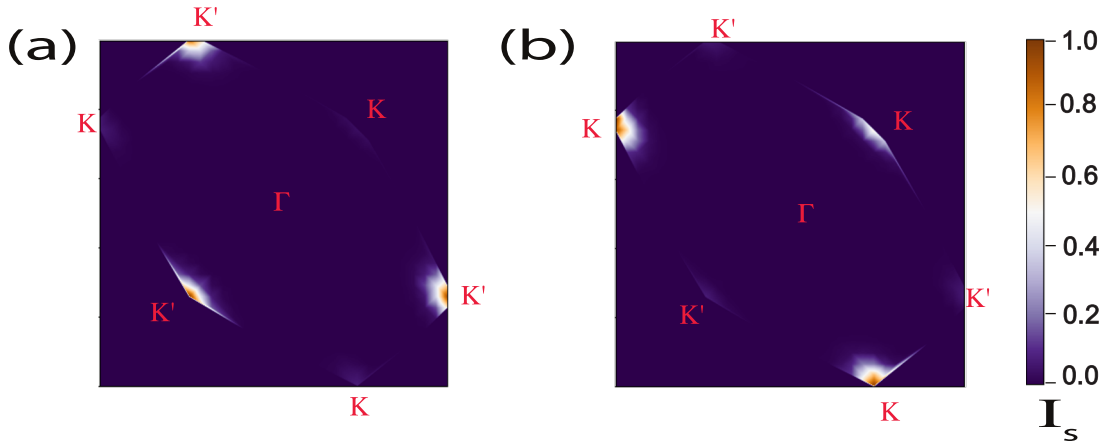

FIG. S3: The oscillator strengths of the first bright singlet (A) exciton in the presence of (a) left and (b) right-handed circular polarized lights.