

Supplemental Material for:
**Optoelectronic Properties and Excitons in Hybridized
Boron Nitride and Graphene Hexagonal Monolayers**

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We show below in two separate figures the bandstructure and the DFT-RPA optical absorption spectra of zig-zag CBN superlattices with a total of 8 rows of atoms in the unit cell (see Fig. 1(b) in the main text). Overall, the zig-zag type monolayers show behavior analogous to the armchair case, namely a tunable band gap that nearly closes at the K point when one residual row of BN is present, and two absorption peaks that red-shift and vary their relative intensity as the C domain size is increased. We note some slight differences compared to the armchair cases, mainly in the different character of the states close in energy to the band gap that attain a higher hybridization between the C and BN for the zig-zag case, and a multivalley bandstructure (seen up to one residual BN row) absent in the armchair case.

In particular, we observe the presence of a band crossing event occurs between the $C_6(BN)_2$ and $C_7(BN)_1$ cases, where during the incipient Dirac cone formation the multivalley structure is removed and a band previously higher in energy and with C character forms a nearly closed Dirac cone in the $C_7(BN)_1$ system at the K point.

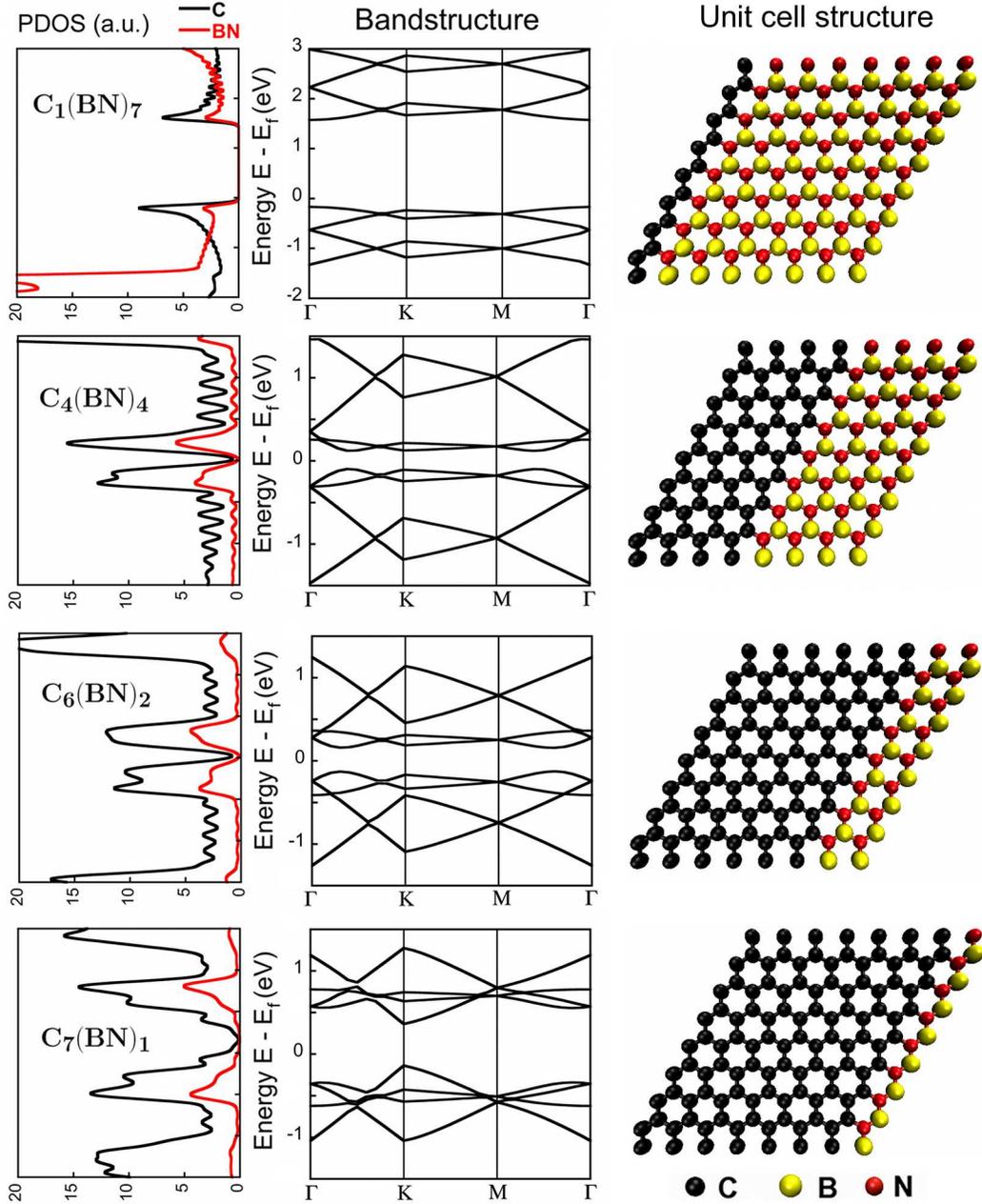


FIG. 1. (color online) PDOS and bandstructure plots of four zig-zag superlattices; the corresponding unit cells used in the calculation are also shown on the right. When the number of C rows is increased (and so is the C concentration), the band gap decreases continuously. However, the Dirac cone typical of graphene only starts forming for one residual BN row, following a sudden change in the bandstructure. The PDOS shows the states close in energy to the gap are mainly due to mixing of C valence states, though the contribution from BN is higher than in the armchair case (see Fig. 2 in the main text).

Absorption spectra: ϵ_2 (a. u.) vs. Energy (eV)

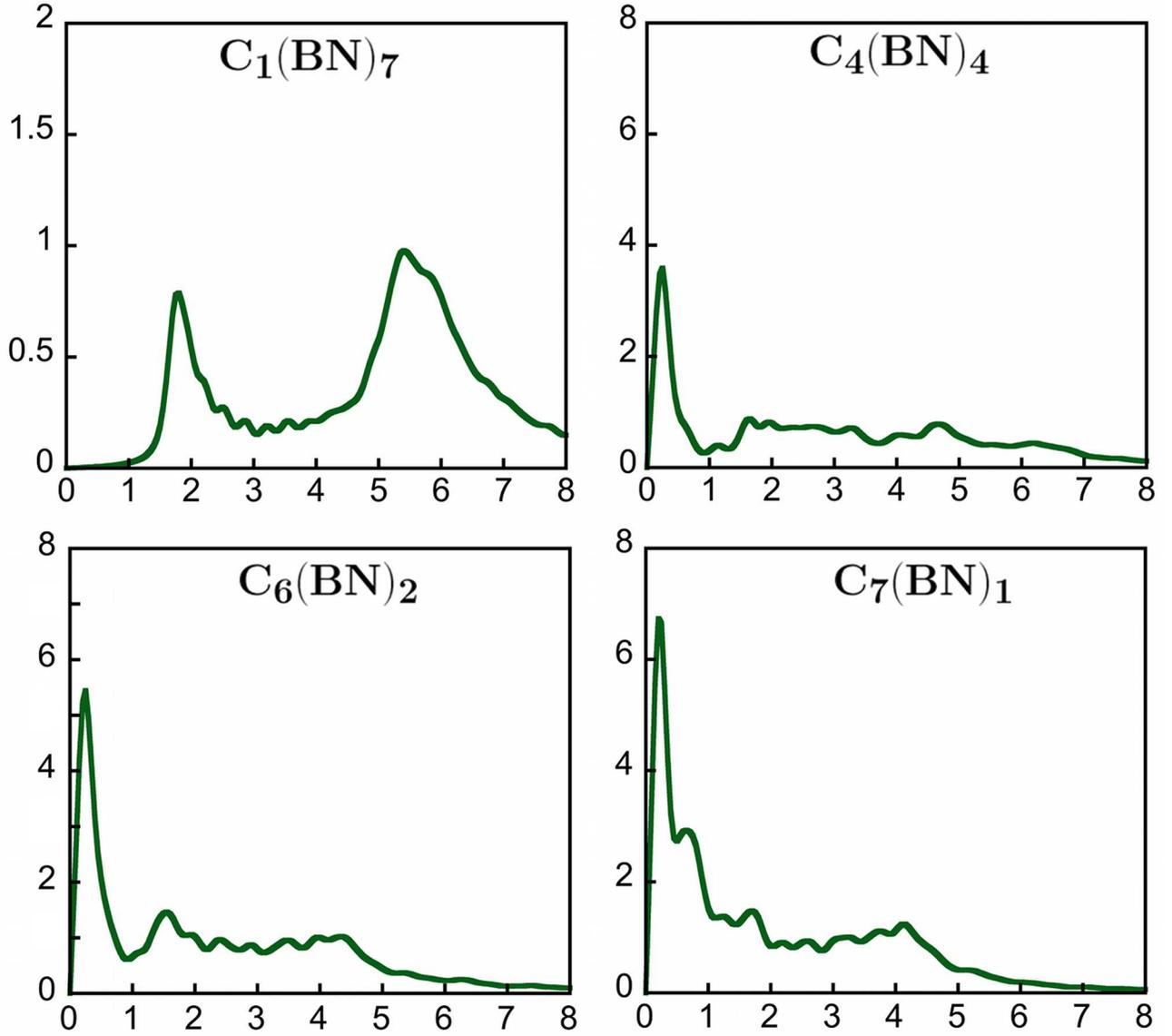


FIG. 2. DFT-RPA optical absorption (expressed as the imaginary part of the dielectric tensor, ϵ_2) of the four zig-zag structures whose bandstructure is shown above. The two absorption peaks red-shift and change their relative strength for increasing C domain size, analogous to the armchair case in Fig. 3(a) of the main text.

We show here further evidence of the dependence of the band gap on C domain size rather than composition for the CBN system. Calculations of the Kohn-Sham band gap of four different systems *with a same C concentration of 50%*, but different C domain sizes are presented in Fig. 3 below.

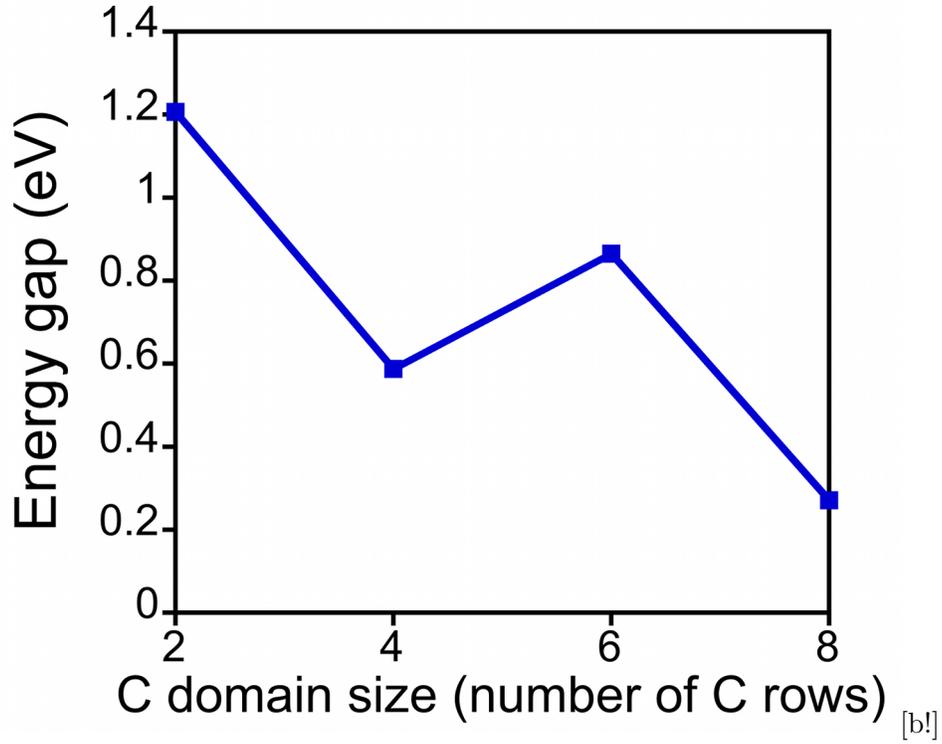


FIG. 3. Band gap of four different structures with the same composition (50% C, 50% BN), but with different C domain sizes. The structures analyzed are $C_2(BN)_2$, $C_4(BN)_4$, $C_6(BN)_6$, and $C_8(BN)_8$, with a C domain size of, respectively, 2, 4, 6, 8 C rows. This plot shows clearly how for a given C concentration, the band gap *is not constant* and rather varies according to the C domain size, which is the main variable regulating the band gap in CBN monolayers.