Supplementary Information for:
Electronic and optical properties in helical trilayer graphene under compression

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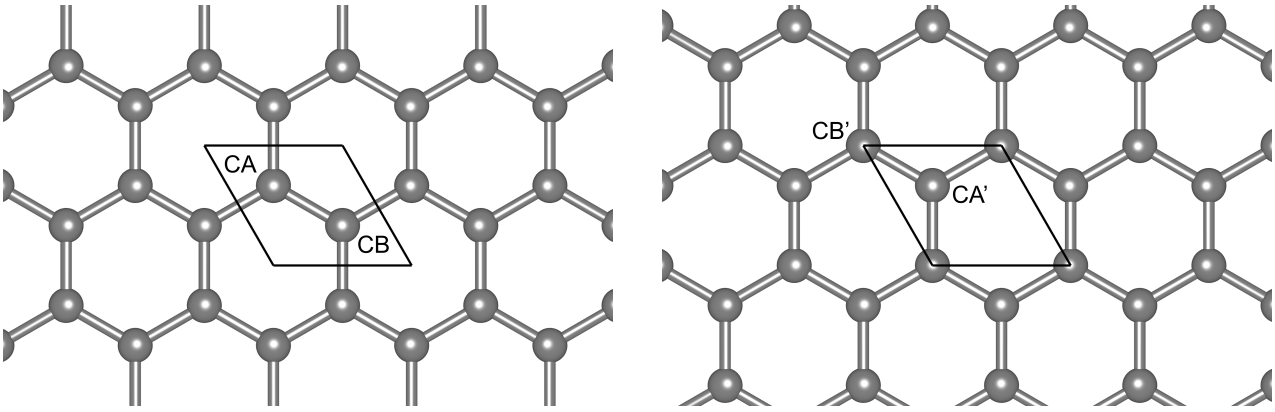
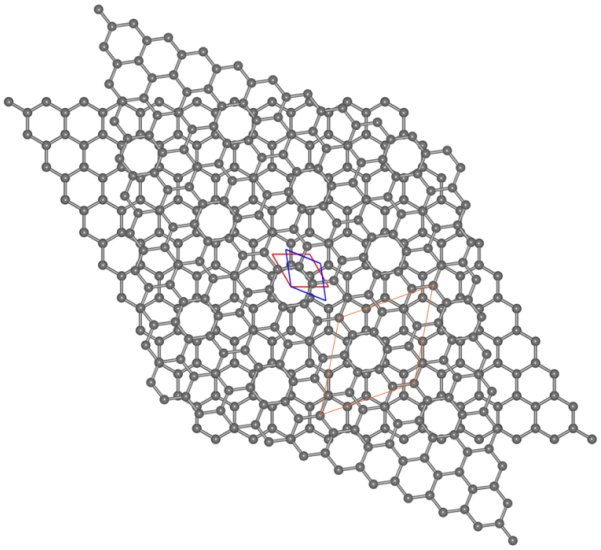
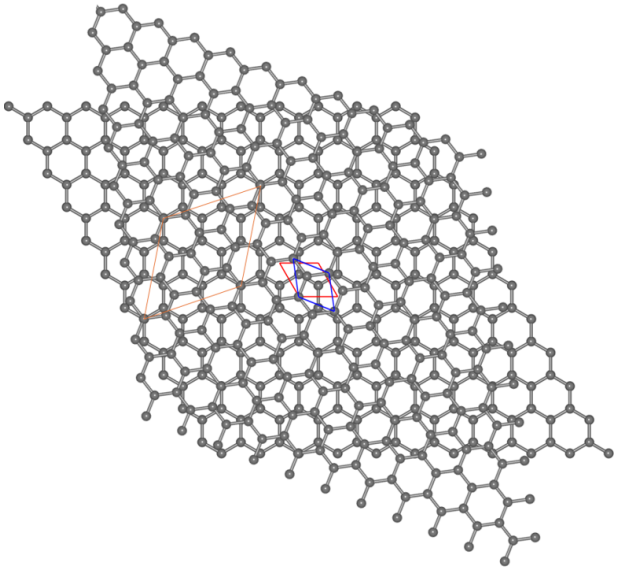


(a) Atomic basis: CA y CB. (b) Atomic basis: CA' y CB'.

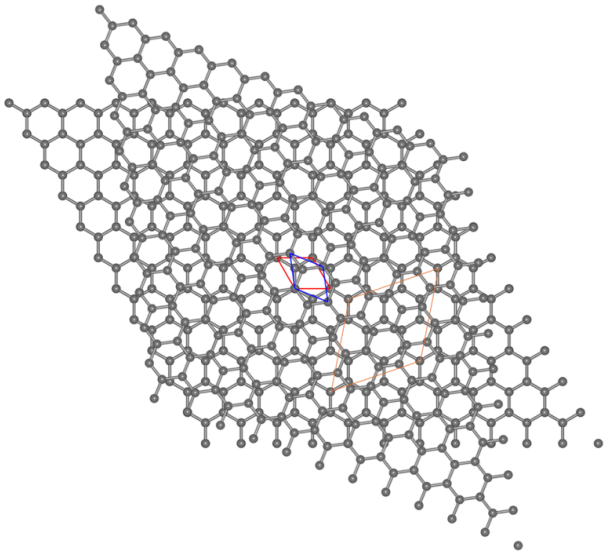
FIG. S1. Hexagonal primitive graphene cells with two different sets of atomic coordinates. Figure (a) shows the first set of CA and CB atomic positions, while figure (b) shows the second set of CA' and CB' atomic positions. See Eq. 3 in the main text.



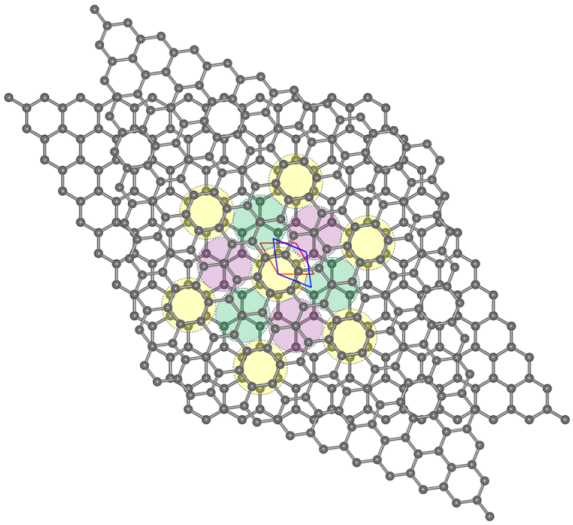
(a) Superposition of two graphene layers with (CA,CB) atomic basis for both red and blue layers. The resulting periodic structure has an even sublattice-exchange parity. C_6 is locally defined in a hexagonal center at the intersection of the red and blue cells.



(b) Superposition of the two graphene layers with the (CA,CB) atomic basis for the red layer and (CA',CB') atomic basis for the blue layer. The final periodic structure has odd sublattice-exchange parity. C_3 is locally defined in the top position of the carbon atom of the blue cell and at the intersection of the red and blue cells.

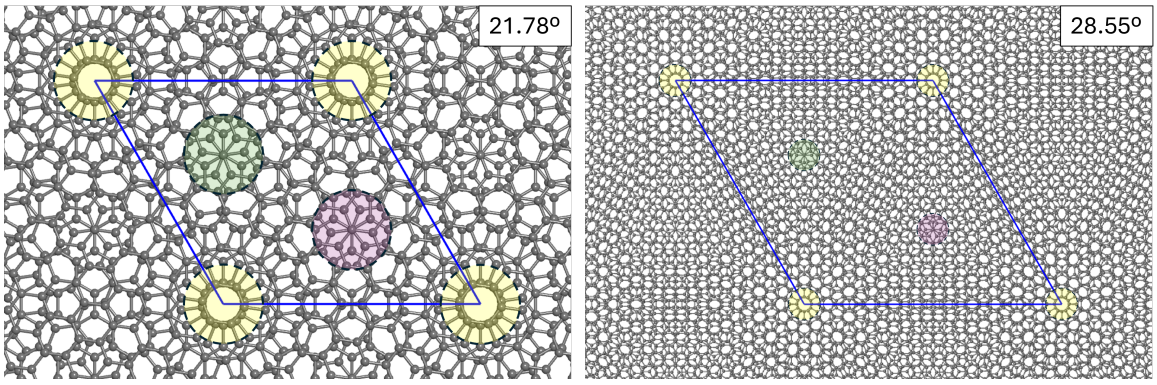


(c) Superposition of the two graphene layers with the (CA',CB') atomic basis for both layers. The resulting periodic structure has odd sublattice-exchange parity. This geometry is equivalent to that in Figure (b) by applying a rotational symmetry, C_{2z}, in 2D. C_3 symmetry is observed locally at the top position of the two carbon atoms of both blue and red cells. The intersection between the red and blue cells at the corners of the hexagons was used as a reference.

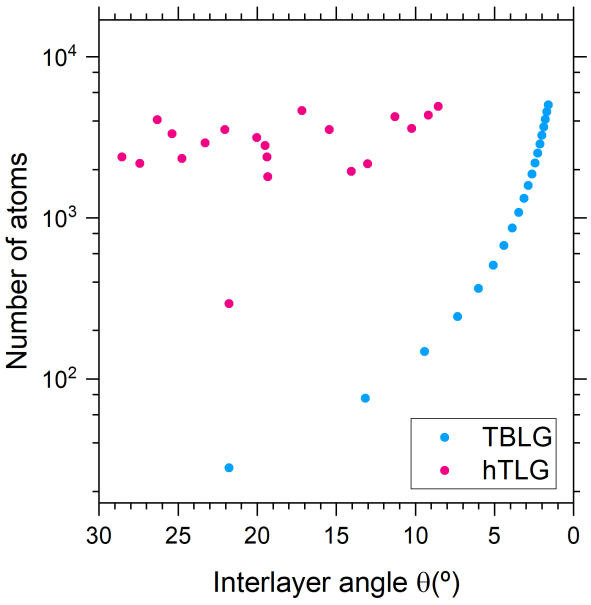


(d) Same system as in Figure (a). Locally, the stacking regions were indicated by the colored regions.

FIG. S2. Twisted bilayer with 21.78°: hexagonal graphene flakes forming a periodic superlattice defined by the orange cells in (a), (b), and (c). The relative orientation can be observed by considering the original red and blue graphene unit cells with different atomic basis positions. Different vertical-stacking regions are identified in (d). The yellow, green, and purple circles denote an AA, AB, and BA stacking, respectively.



(a) Top view of the two periodic hTLG systems. The colored regions follow the same notation as in Figure S2(d).



TBLG [θ]	TBLG - Natoms	hTLG [$\theta_1 = -\theta_2$]	hTLG - Natoms
21.79	28	28.55	2388
13.17	76	27.42	2178
9.43	148	26.32	4066
7.34	244	25.39	3342
6.01	364	24.76	2345
5.09	508	23.29	2930
4.41	676	22.06	3530
3.89	868	21.79	294
3.48	1084	20.03	3150
3.15	1324	19.50	2816
2.88	1588	19.35	1804
2.65	1876	17.17	4644
2.45	2188	15.46	3532
2.28	2524	14.06	1948
2.13	2884	13.02	2166
2.00	3268	19.39	2396
1.89	3676	11.29	4258
1.79	4108	10.25	3602
1.70	4564	9.19	4342
1.61	5044	8.56	4918

(b) Total number of atoms as a function of the interlayer angle for helical trilayer graphene (hTLG) systems and twisted bilayer graphene (TBLG) for comparison.

FIG. S3. (a) Atomic models of the hTLG-1 system with $\theta_1 = 21.78^\circ$ and the hTLG system with $\theta_1 = 28.55^\circ$ are shown for visual comparison. (b) Results obtained for twisted helical trilayer graphene systems with several different interlayer angles θ_1 and θ_2. The constraint to build the helical structures is $\theta_1 = -\theta_2$.

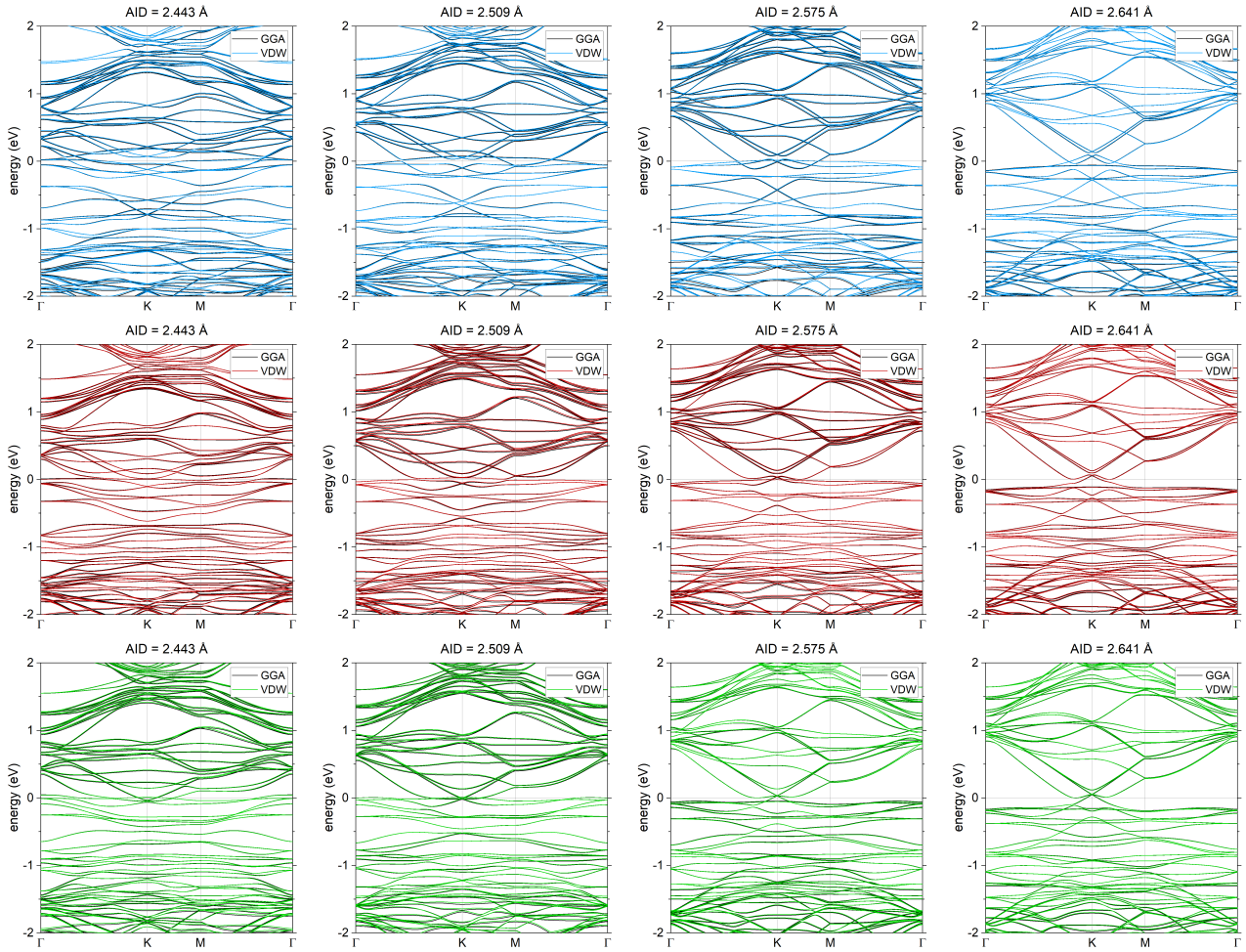


FIG. S4. Electronic band structures calculated with different exchange-correlation approximations (GGA-PBE and VDW-KBM) and at different average interlayer distance (AID). The set of blue, red and green band structures are for the hTLG-1, hTLG-2 and hTLG-3 systems, respectively. Notice that, the dispersion relations with GGA and VDW are identical. The Fermi energy is at 0 eV.