Supplementary Information

Point Defects in Turbostratic Stacked Bilayer Graphene

Chuncheng Gong[1], Sungwoo Lee[2], Suklyun Hong[3], Euijoon Yoon[2], Gun-Do Lee[2,], Jamie H. Warner[1,*]*

[1]Department of Materials, University of Oxford, Parks Road, Oxford, OX1 3PH, United Kingdom

[2]Department of Materials Science and Engineering, Seoul National University, Seoul, 151-742, Korea

[3]Department of Physics and Graphene Research Institute, Sejong University, Seoul 143-747, Korea

Corresponding author: gdlee@snu.ac.kr (Gun-De Lee); jamie.warner@materials.ox.ac.uk (Jamie H. Warner)

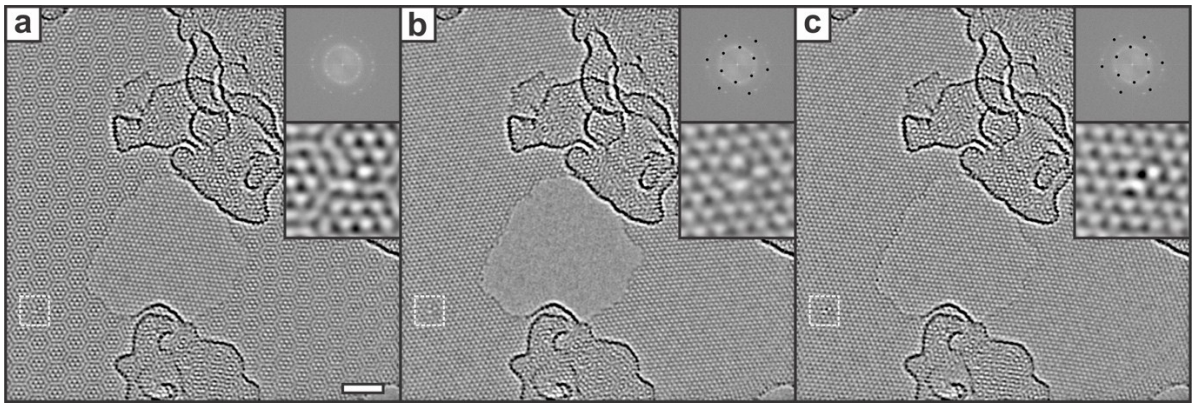

Figure S1. AC-TEM image of a 555-777 DV_2 in turbostratic stacked bilayer graphene. (a) AC-TEM image of the bilayer graphene with its FFT and magnified view of the area cropped by the white dashed square shown in the insets. (b,c) The two layers are separated by placing a negative mask on one of the two sets of hexagonal patterns in the FFT. The scale bar in panel a is 2 nm.

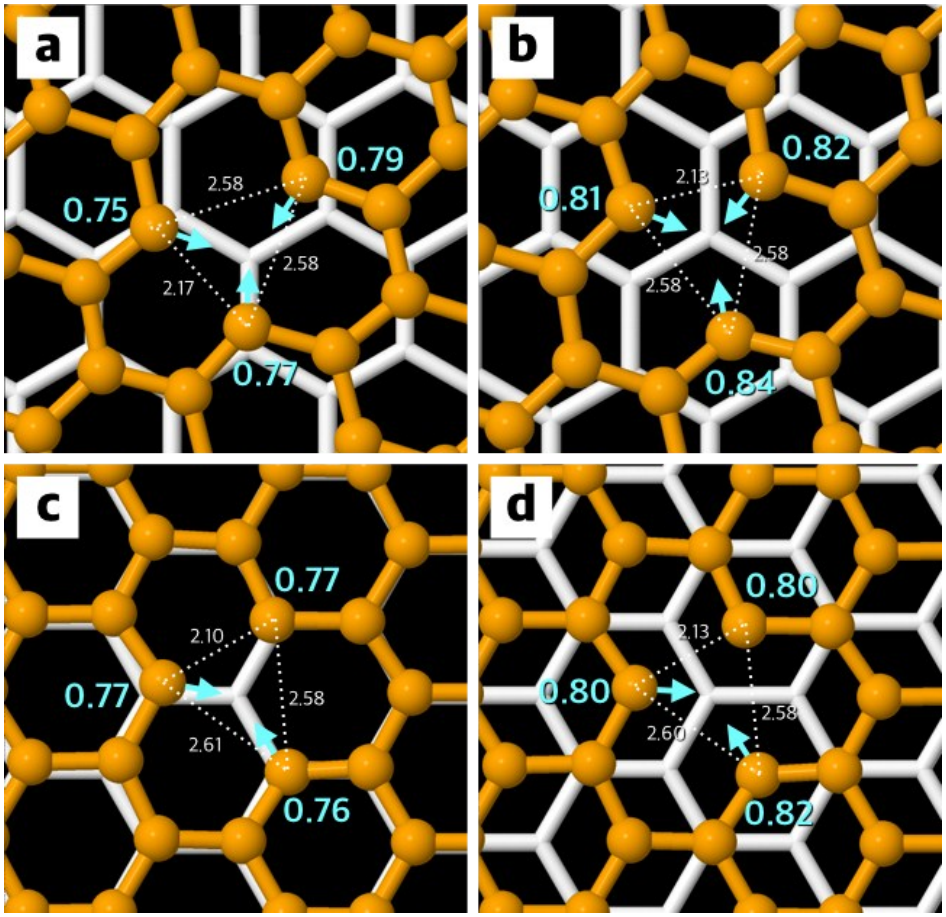

Figure S2. Diffusion barriers of atom in bilayer graphene of 13.2° mismatch angle (a, b), in AA (c) and AB (d) stacked bilayer graphene Blue arrows indicate the direction of atom diffusion and blue numbers indicate the diffusion barriers. White small numbers indicate the bond lengths of C-C. The atomic arrangement nearby vacancy in AA stacking bilayer graphene (c) is very similar to that in (a). The atomic arrangement nearby vacancy in AB stacking bilayer graphene (d) is very similar to that in (b). The diffusion barriers in (c) are very similar to (a) and the diffusion barriers in (d) are very similar to (b).

Energy (eV)	Γ only	3x3x1	4x4x1	6x6x1
MV migration (atom 1)	0.79	0.76	0.75	0.75
MV migration (atom 3)	0.83	0.80	0.79	0.79

Table S1. Convergence test of diffusion barriers of atoms depending on k-point sampling. Atom 1 and 2 are corresponding to atom 1 and 2 in Figure 5b. From 4x4x1 k-point sampling, the diffusion barriers are almost converged. The difference between two diffusion barriers are same as 4 eV regardless of k-point sampling.

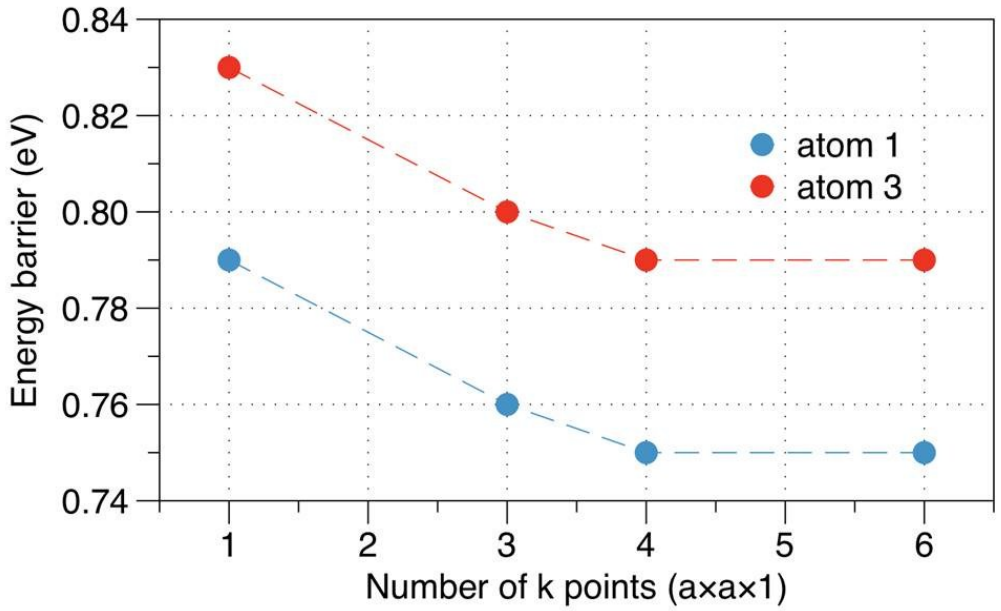

Figure S3. Curves showing the convergence test of diffusion barriers of atoms depending on k-point sampling from Table S1.

Movie S1 : Movie from TBMD simulation which confirms the structural change from Figure 6 (m) to (o)