Electronic Supplementary Material (ESI) for Nanoscale.

Supplementary Information

Detailed Formation Processes of Stable Dislocations in Graphene

Gun-Do Lee[1*], Euijoon Yoon[1], Kuang He[2], Alex W. Robertson[2], Jamie H. Warner[2*]

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

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

*Email : gdlee@snu.ac.kr (Gun-Do Lee), jamie.warner@materials.ox.ac.uk (Jamie H. Warner)

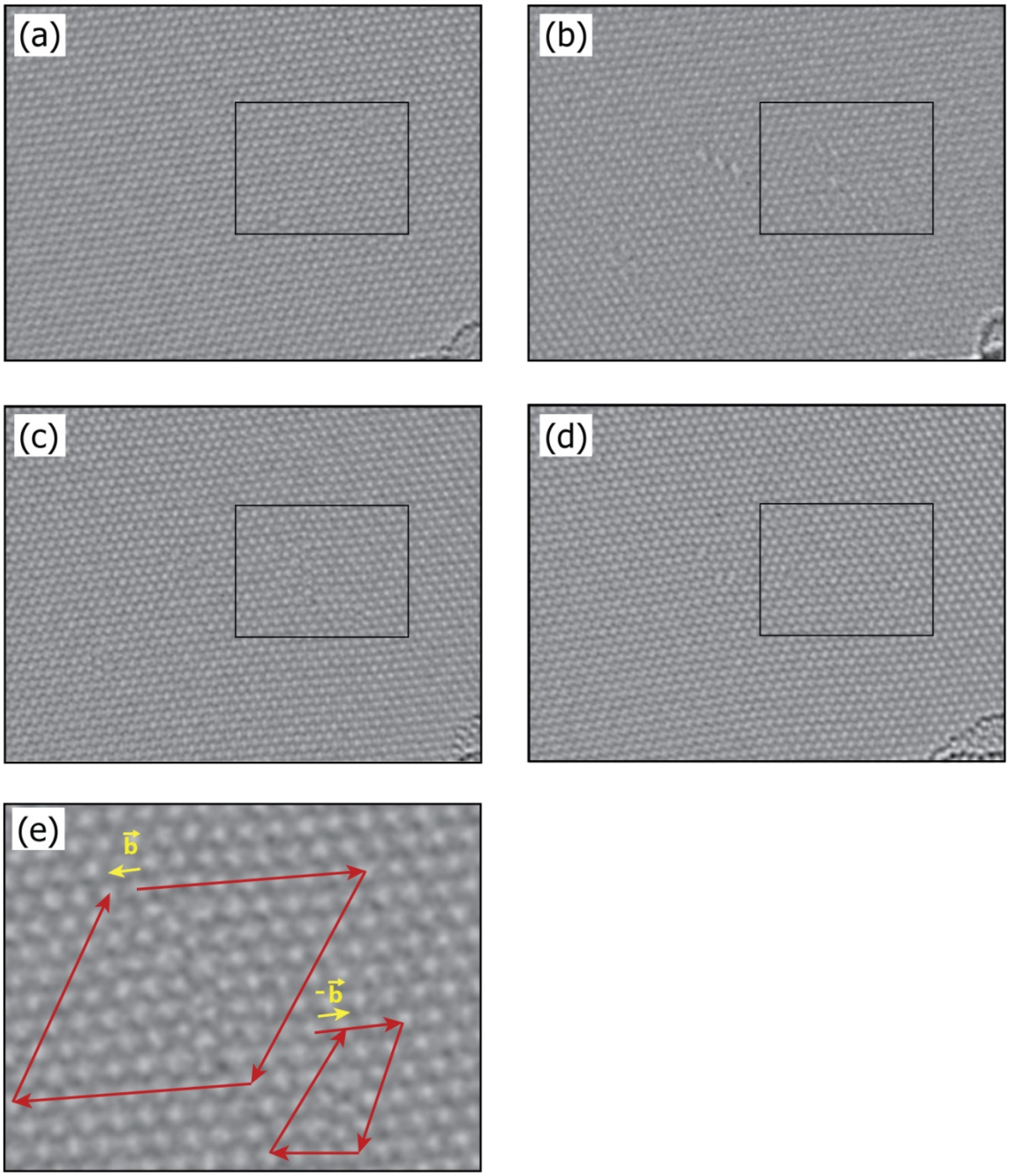

Figure S1. (a)-(d), HRTEM images of stable dislocation formation. Square in each panel is same area and corresponds to the frames of Figure 1. Graphene is first exposed to a 80 kV focused electron beam for 1 minute to create the initial defects imaged in a. Then the electron beam was focused again for 5 minutes. Image b was taken right after the 5 minutes of focused electron beam irradiation. Defect structures are not clearly identified due to large defocus. Image c was taken one minute later from b. Figure 1a in the main text is an

enlarged image of the square in c. d is the final image taken after 362 sec from a and Figure 1h in the main text. Figure 1h is an enlarged image of square in d. See supporting movie S1 for whole process. (e), Formation of two dislocations shown in the image of Figure 1a. Two burgers vectors are opposite each other. It shows the inter-connection of two dislocations because those are formed from evaporation of carbon atoms and total burgers vector is zero.

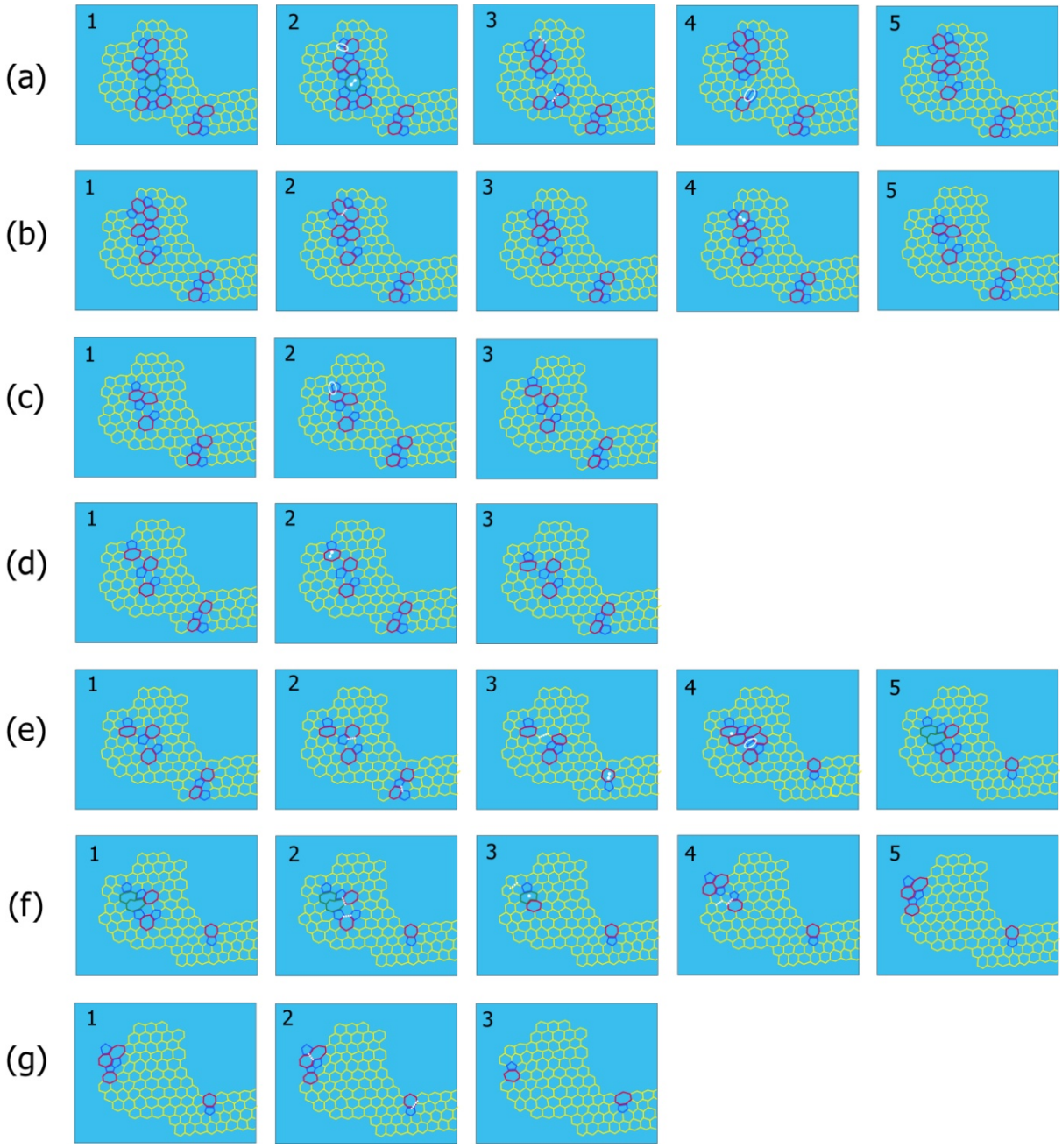

Figure S2. Suggested models for possible reconstruction processes from Figure 1a to Figure 1h. White dotted lines indicate carbon-carbon bonds undergoing SW type bond rotation at the next step. White dumbbells and dots indicate adsorbed dimer and atom, respectively. White ellipses indicate the evaporated dimer at the next step. Figures at first column of a-g are corresponding to structural models of Figure 1a-g, respectively. The rightmost figure in g is corresponding to the structural model of Figure 1h. In the process of transformation shown in a, the system undergoes two SW type bond rotations (a-3), the adsorption of one dimer (a-2),

and the evaporation of two dimers (a-2 and a-4). From a-4 to a-5, due to the evaporation of a dimer, the 5-7 pair is observed to climb. In b, the number of non-hexagonal rings is reduced by the SW type bond rotation (b-2) and the adsorption of carbon dimer in heptagon (b-4). In c, a dimer is evaporated, which induces the separation of two 5-7 pairs as shown in c-3. In d, a dimer is adsorbed at a heptagon and it causes the motion of 5-7 pair compared with c. The process in e is fully explained in main text and Figure 3. In e, non-hexagonal rings are significantly increased with adsorption of adatom as shown in e-5. In f-2, two SW type bond rotations reduce dramatically the number of non-hexagonal rings. In f-3, an adatom is adsorbed and combines with the atom adsorbed in e4 for many non-hexagonal rings to be altered into a 5-7 pair finally as shown in f-4. By electron irradiation, a SW defect is also formed nearby the 5-7 pair as shown in f4 and it coalesces with a 5-7 pair by two SW type bond rotation as shown in f-5. In g, the SW defect is altered into hexagons due to the SW type bond rotation and a dislocation pair with two 5-7 pairs is formed. These reconstruction processes are suggested to connect two successive HRTEM images. The SW type bond rotation, the evaporation of dimers, and the adsorption of dimers and adatoms should exist to explain the reconstruction processes although the order may be different with real processes. From the analysis, we can count the number of evaporated atoms and adsorbed atoms during the process. In a, two atoms are lost by the evaporation of two dimers and adsorption of one dimer. In b, two atoms are added by the adsorption of one dimer. In c, two carbon atoms are lost by the evaporation of one dimer. In d, two carbon atoms are added by the adsorption of one dimer. In e, one carbon atom is added by the adsorption of one dimer and one atom and by the evaporation of one dimer. In f, one atom is added. In g, there is no change in the number of atoms. Therefore, total two carbon atoms are added during the process from a to g.

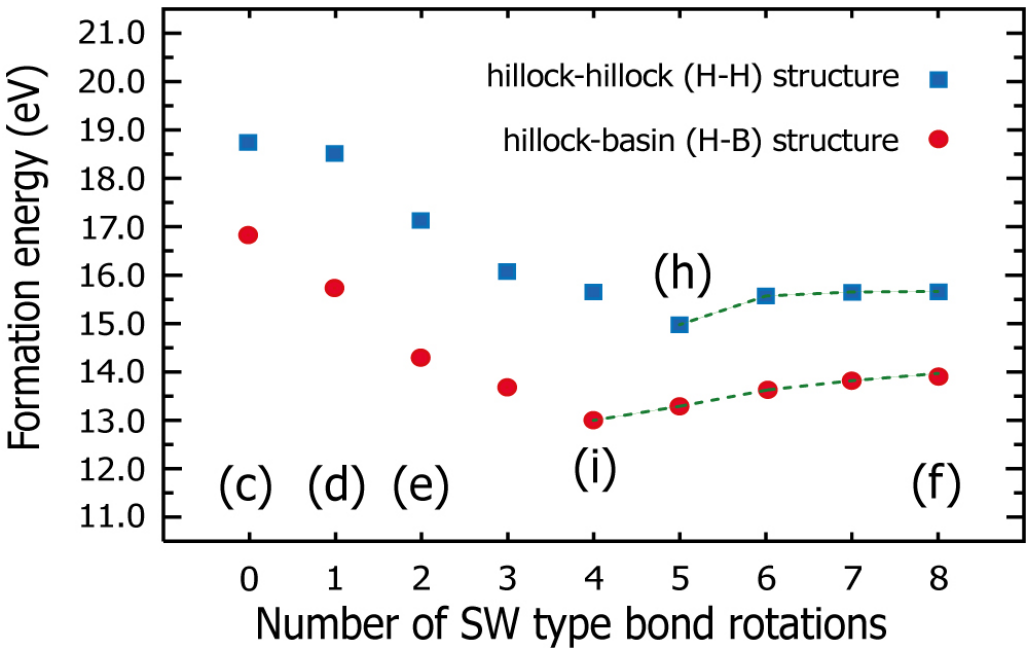

Figure S3. The formation energies of dislocation pair with two 5-7 pairs from Figure 3c to 3f from DFT calculation

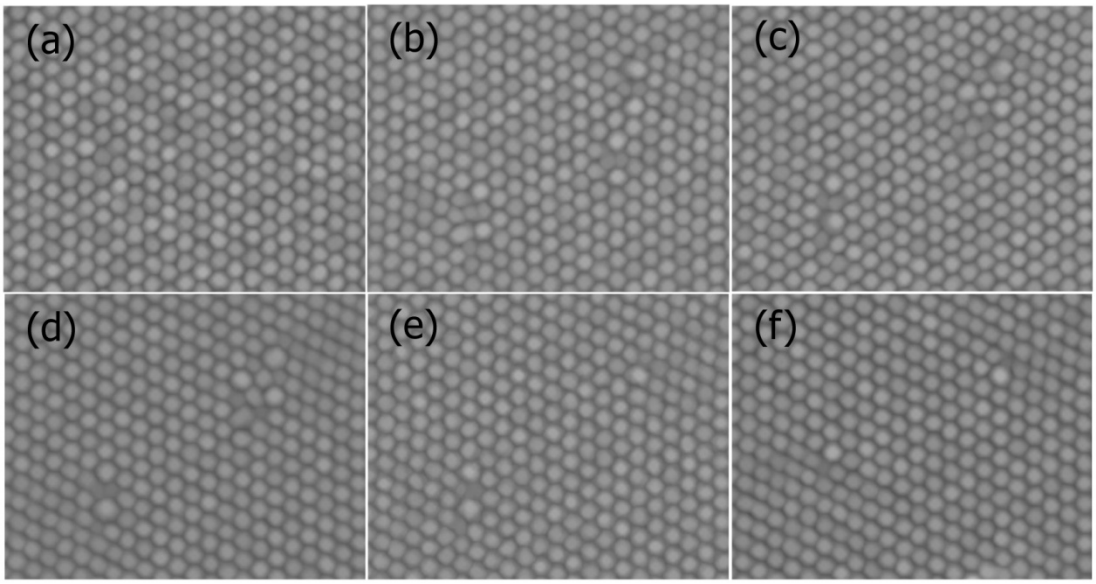

Figure S4. Non-annotated HRTEM images of Figure 4 after smoothing and a maximum filter is applied.

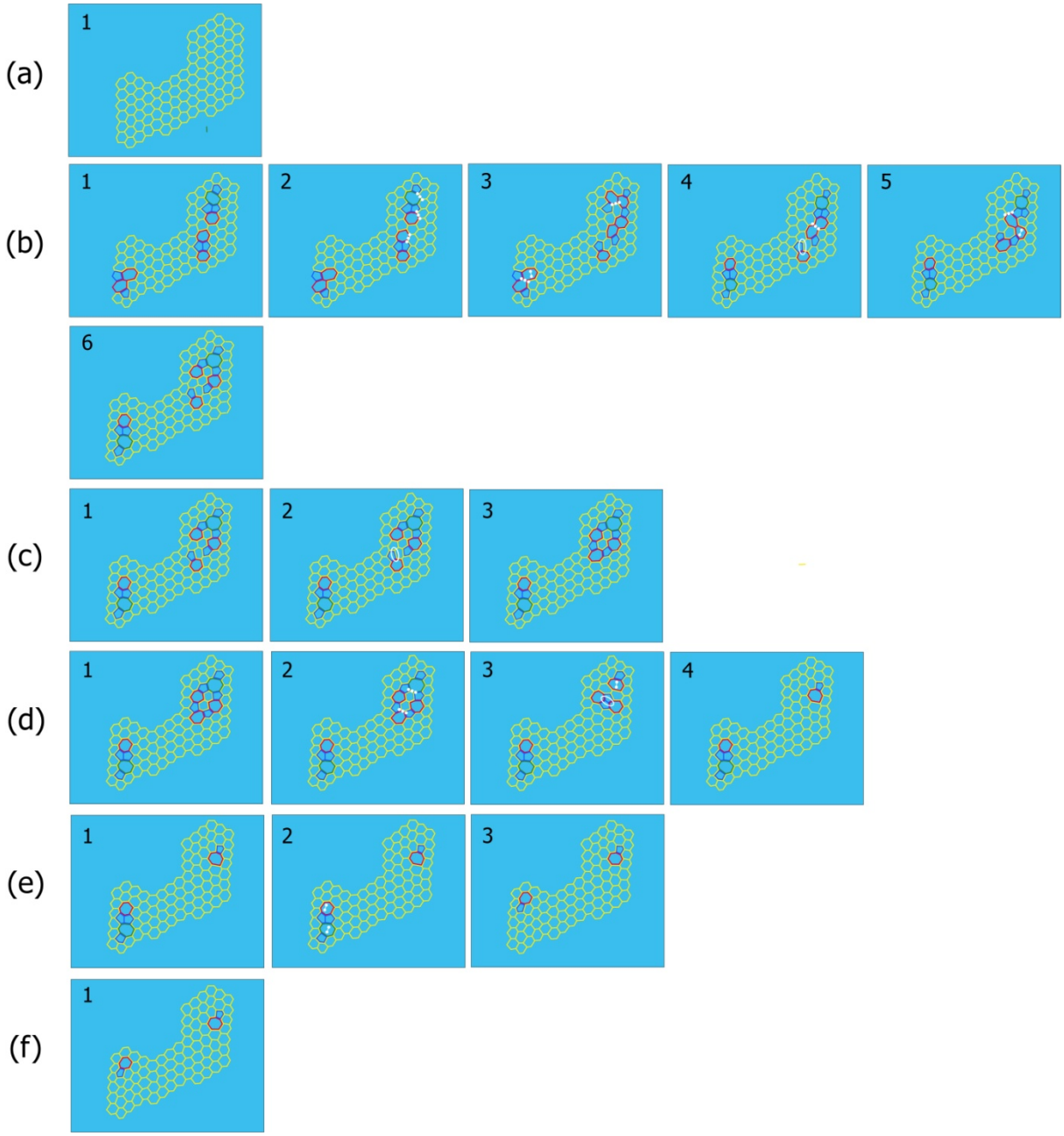

Figure S5. Suggested models for possible reconstruction processes from Figure 4a to Figure 4f. White dotted lines indicate carbon-carbon bonds undergoing SW type bond rotation at the next step. White dumbbells and dots indicate adsorbed dimer and atom, respectively. White ellipses indicate the evaporated dimer at the next step. Figures at first column of a-f are corresponding to structural models of Figure 4a-f, respectively.

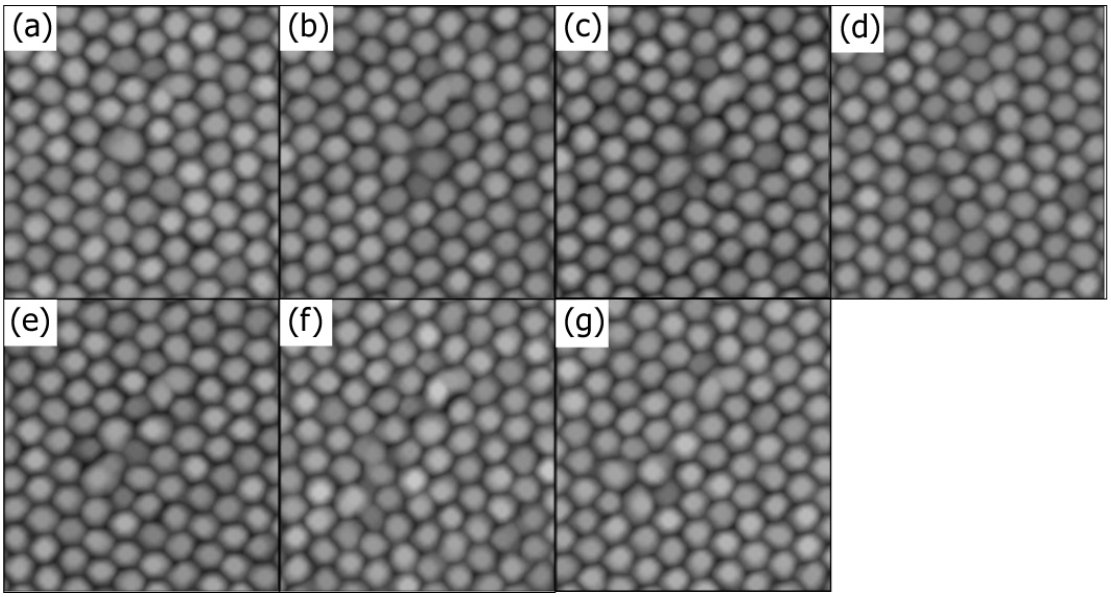

Figure S6. Non-annotated HRTEM images of Figure 5 after smoothing and a maximum filter is applied.