Electronic Supplementary Material (ESI) for Chemical Communications

Tailoring on-surface supramolecular architectures based on adenine directed self-assembly

Supporting Information

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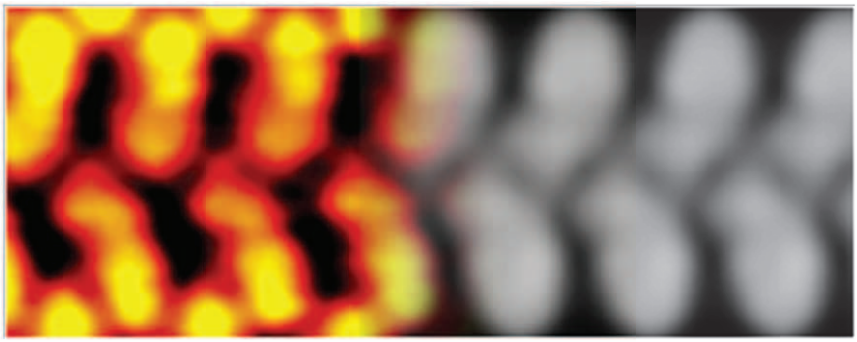

Figure S1. The ribbon structure of BPA molecule shown in Figure 1a (left panel) overlaid with the corresponding STM image simulation (right panel) in the bias condition of 1.05 V which is consistent with the experimental condition.

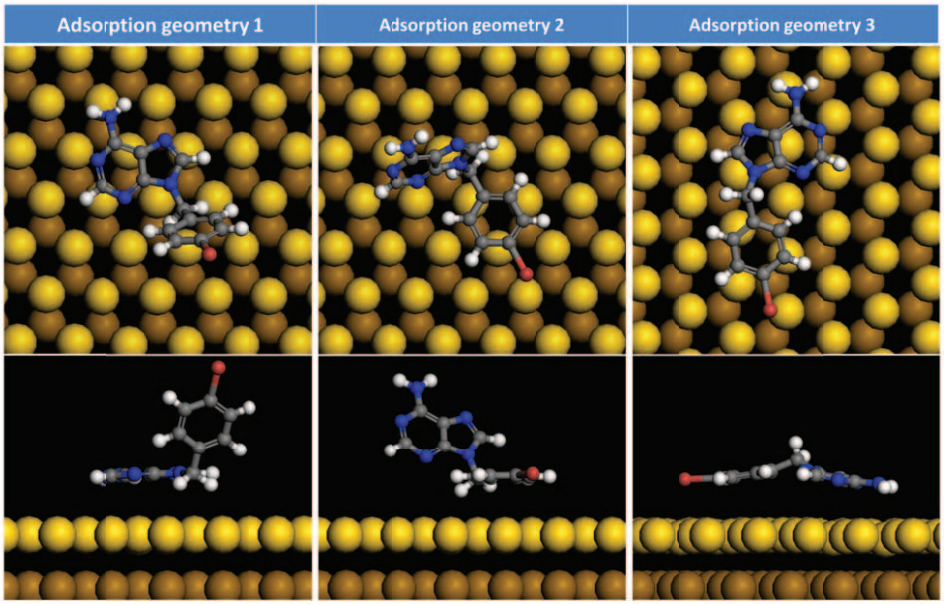

Figure S2. Three different adsorption geometries of BBA molecule on the Au(111) substrate. Adsorption geometry 3 is the most stable one which may be influenced by the surface adsorption, followed by adsorption geometry 1 and adsorption geometry 2 is the most unstable one. Nevertheless, this geometry 3 has not been observed from the STM images, which may be due to: (1) the energetics of the whole self-assembled molecular network structures where the intermolecular interaction may counter-balance the molecule-substrate interaction; (2) the molecular density which may have certain influence as the overall surface adsorption energy of geometry 1 may be higher even the energy per molecule is lower. Also, note that the single molecule in the STM image looks like a bright oval connected with a dark triangle, the adsorption geometry 3 with the only tilted CH2 group is expected to show as a long dark oval with a bright dot at the center, which does not match with the case seen from

the STM image. Thus we believe the intermolecular interactions and the molecular density become dominant when molecules self-assembled into the network structures at higher temperatures where adsorption geometry 1 is the favorable one.

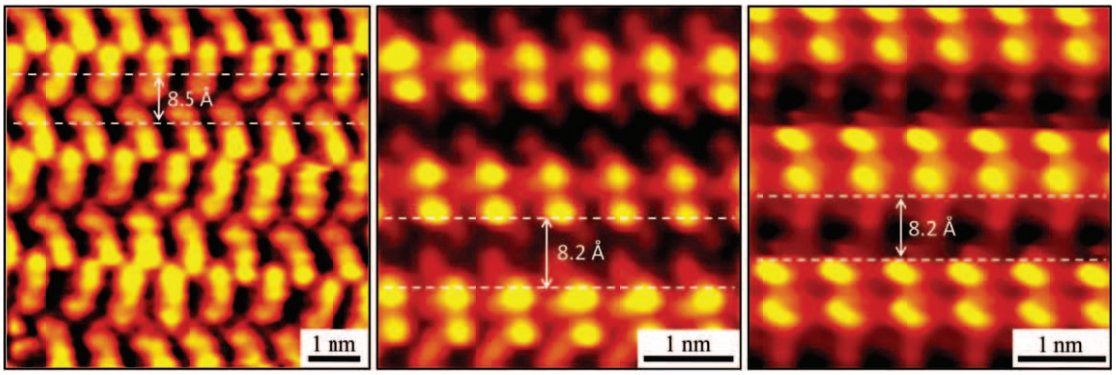

Figure S3. The separations of white dotted lines (i.e. adenine-directed ribbons) have been measured to be 8.5 Å, 8.2 Å and 8.2 Å for structures shown in Figure 1a, Figure 2a and Figure 2b, respectively.

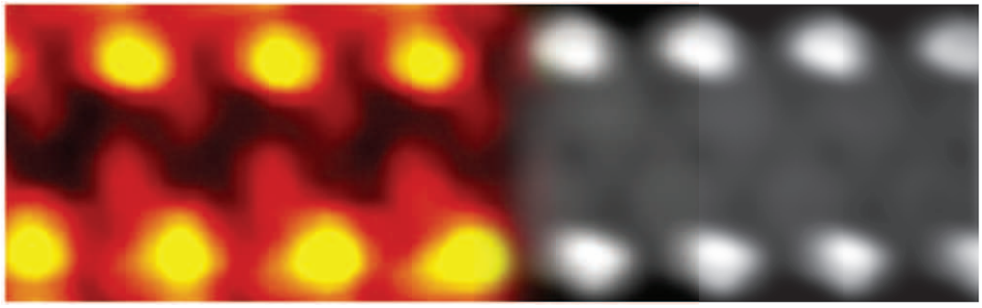

Figure S4. The ribbon structure of BBA molecule shown in Figure 2a (left panel) overlaid with the corresponding STM image simulation (right panel) in the bias condition of 1.05 V which is consistent with the experimental condition.

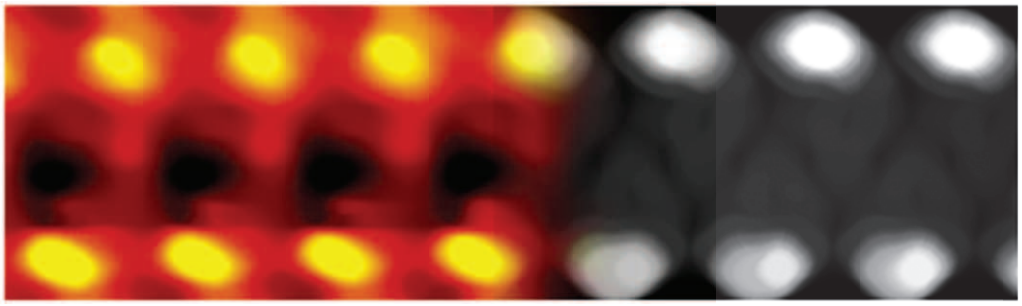

Figure S5. The ribbon structure of BBA molecule shown in Figure 2b (left panel) overlaid with the corresponding STM image simulation (right panel) in the bias condition of 1.05 V which is consistent with the experimental condition.

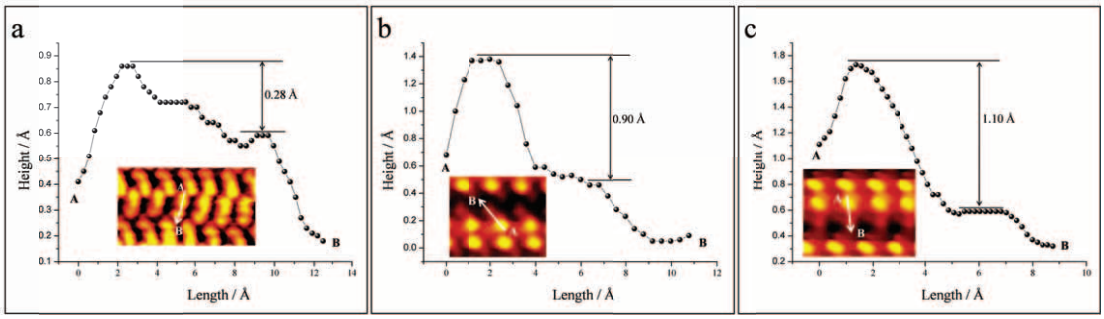

Figure S6. Line profiles across the whole molecule of (a) BPA and (b)-(c) BBA in the corresponding self-assembled structures (cf. Figure 1a, Figure 2a and 2b, respectively). From the height profiles, it can be seen that for the BPA molecule, the line profile across the whole molecule shows the height difference of about 0.28 Å (considering that the Br atom has higher contrast in the STM image), consistent with the nearly flat-lying model. For the homochiral phase of BBA molecule shown in Figure 2a, the height difference is about 0.90 Å, while 1.1 Å for the heterochiral phase shown in Figure 2b. It can be explained by the different angles of the phenyl rings away from the adenine plane demonstrated in the theoretical models as the molecule in heterochiral phase adopts a much more perpendicular geometry.