Electronic Supplementary Material (ESI) for Chemical Communications

Supporting information

Steering Supramolecular Pattern by Nucleobase-Terminated Molecules

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Molecular modeling

Tentative molecular modeling was performed by using Materials Studio and the results were shown in figure S2 and figure S3. In call cases, molecules were packed by estimating that the distance between the two arms (alkyl side chain) is 4.5 Å, and the hydrogen bonding distance is 1.9 Å.

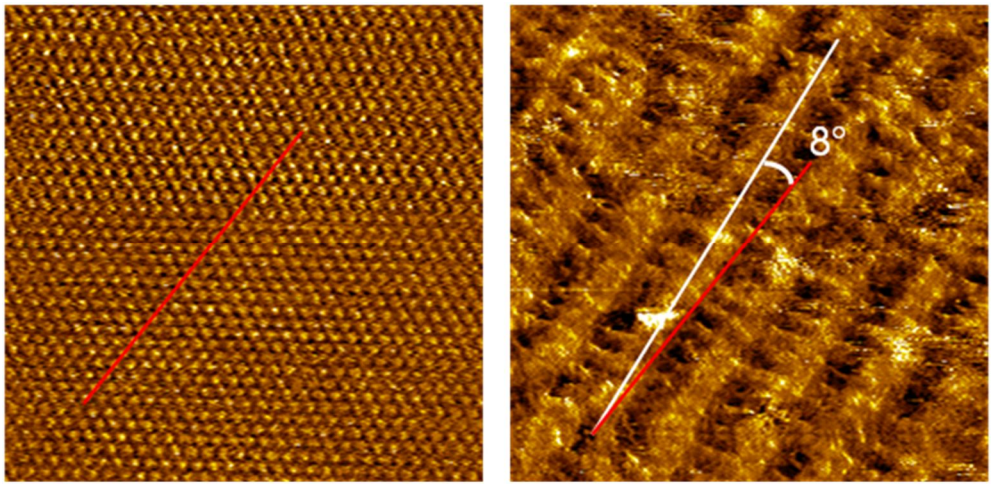

Figure S1. STM image of atomic resolved HOPG surface and A-A dimer on HOPG. The angle between the packing direction of the molecule (indicated by the white line) and the symmetric axe of graphite (indicated by the red line) is 8°.

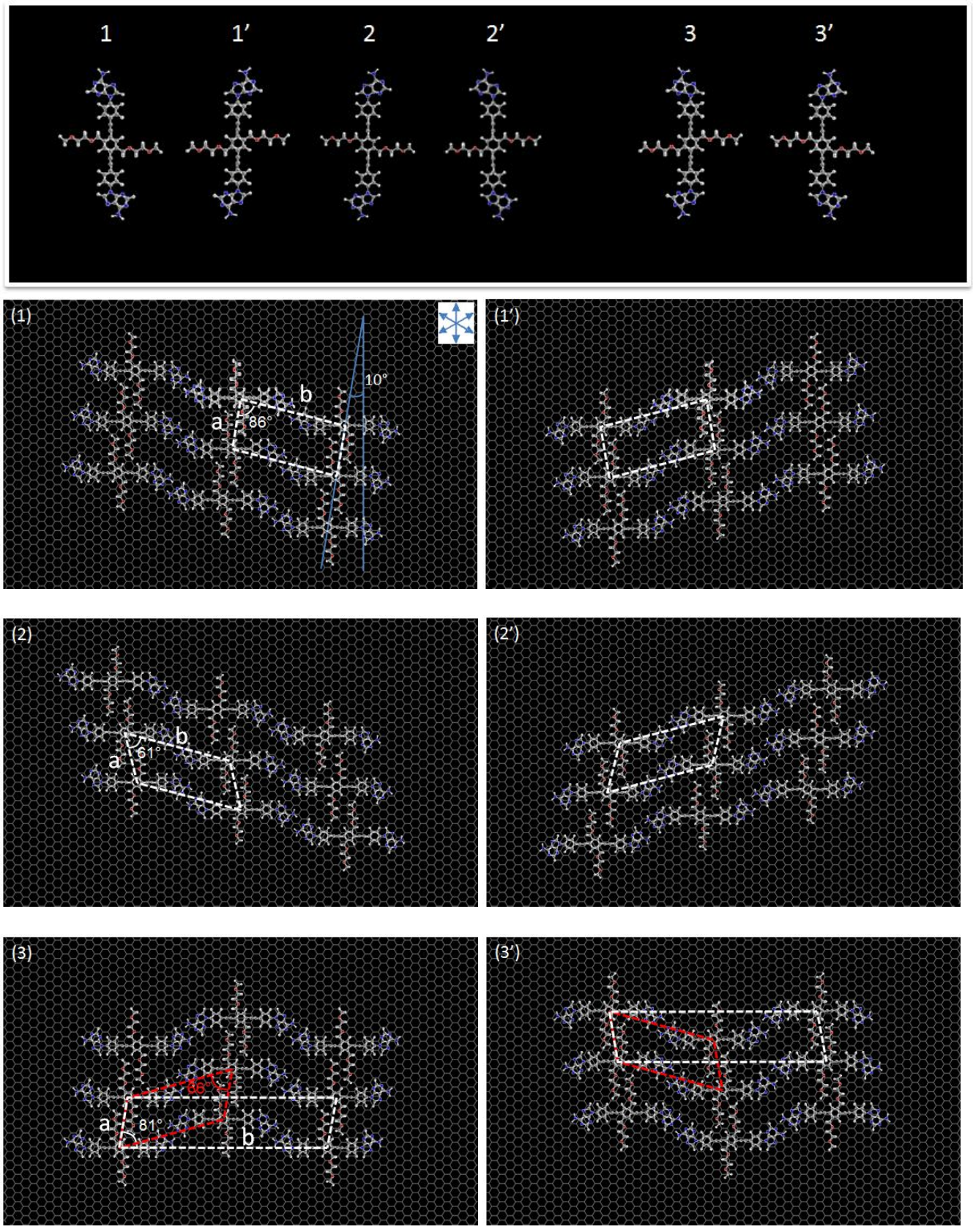

Figure S2. Tentative molecular models indicating possible arrangements of the six conformers of A-A dimer on HOPG (red: O, blue: N, white: H. Only the first layer of HOPG is shown). The unit cell indicated in **1** and **1'** is (13.8×29.3 Å)*R*86°.

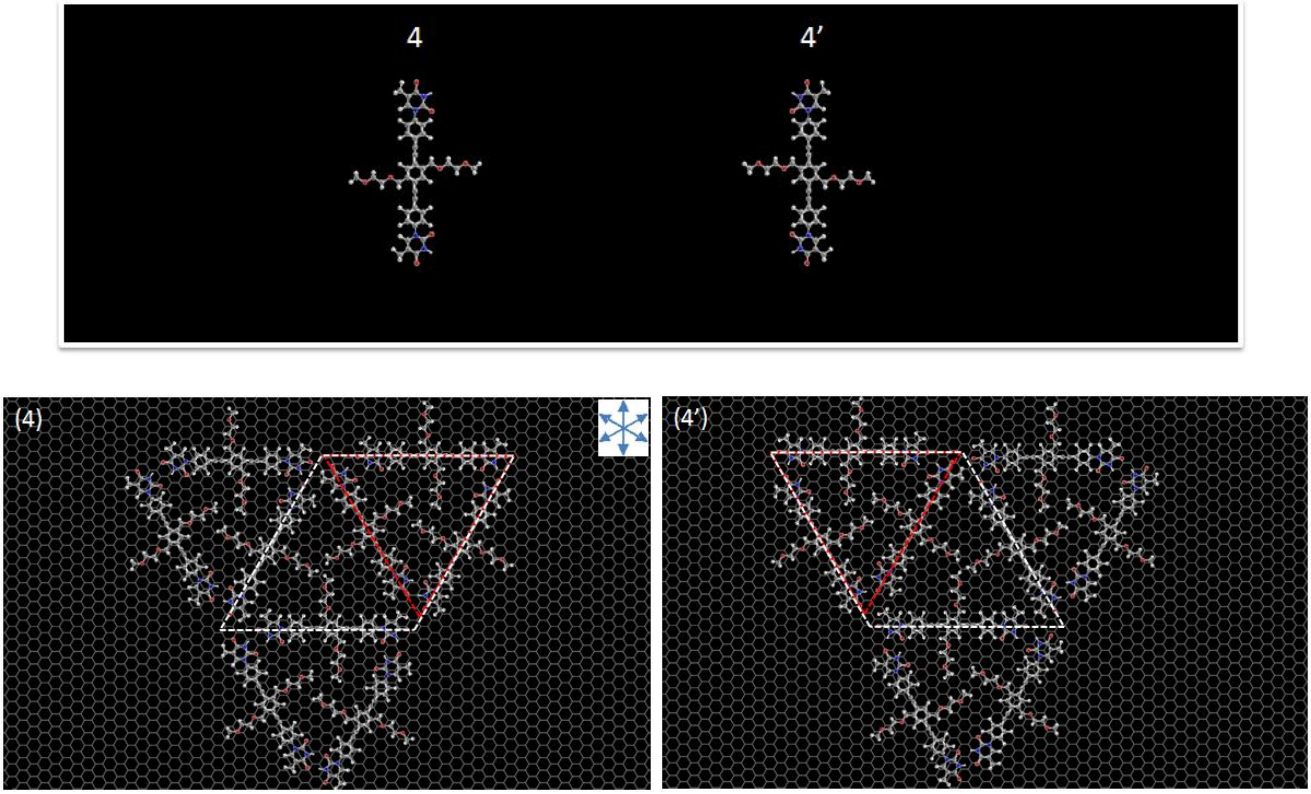

Figure S3. Tentative molecular models indicating possible arrangements of the two conformers of the T-T dimer on HOPG (red: O, blue: N, white: H. Only the first layer of HOPG is shown). The white unit indicates the unit cell. The red unit indicates that the unit cell has a structure of (35.4×35.4 Å)*R*60°.