

Supporting Information

Dynamic Study of binary Network Structural Change in Response to Guest Inclusion

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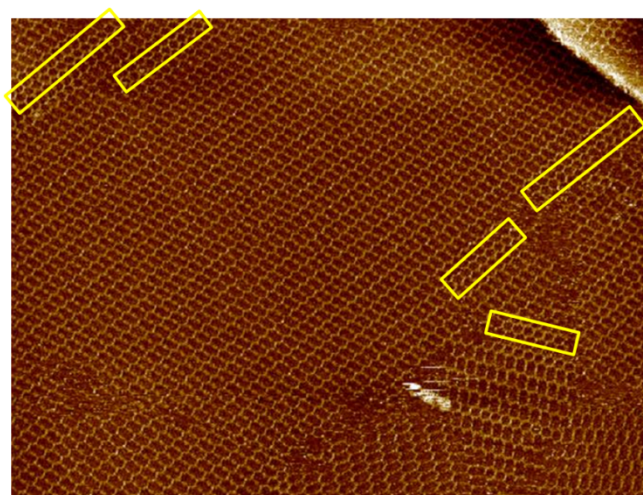


Figure S1. STM image of TMA/Bpy network at the 1-heptanoic acid/graphite interface when the ratio of Bpy to TMA is slightly less than 3:2. The comparatively narrow row in the monolayer highlighted by the yellow square formed from pure TMA network.

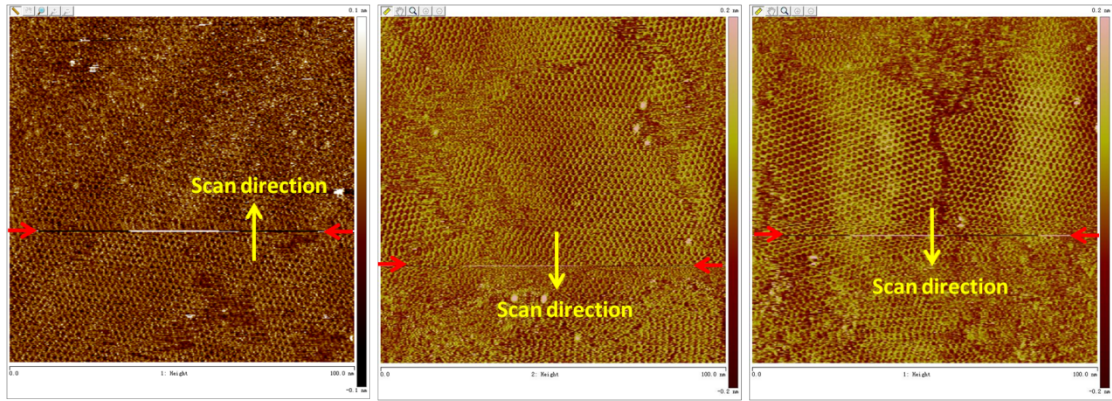


Figure S2. *In-situ* STM imaging the disturbance of COR molecules to the host network (for different experiments). The disturbance line highlighted by two red arrows in each image indicates where the COR was added in situ during scanning.

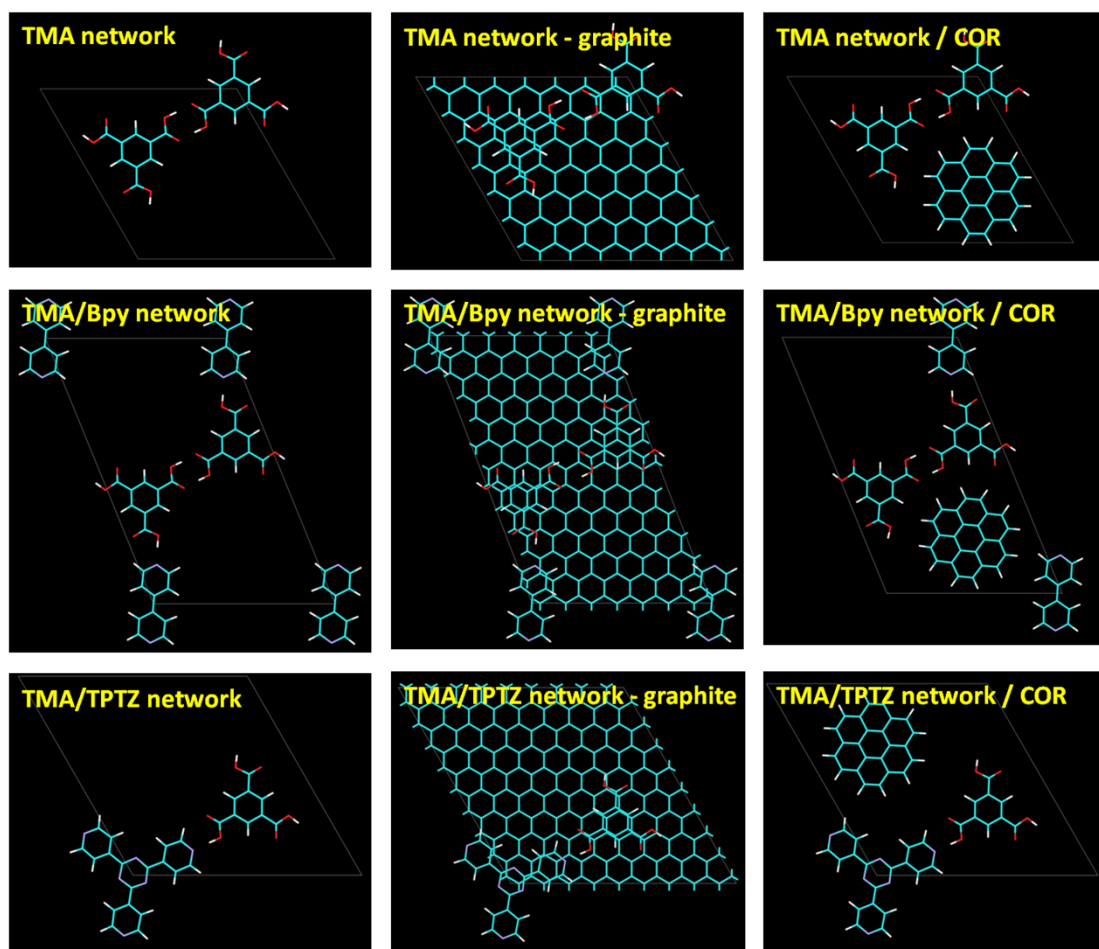


Figure S3: Calculated interaction models of physisorbed molecules with and/or without graphite [1].

[1] In this work, TMA, Bpy, TPTZ and COR molecules are consistent with benzene-ring π -conjugated structures. Because adsorption of benzene on graphite and graphene should be very similar, we have performed our calculations on infinite graphene monolayers using periodic boundary conditions (PBC). In the superlattice, graphene layers were separated by 20 Å in the normal axis direction and represented by orthorhombic unit cells containing two carbon atoms. When modeling the TMA, TMA/Bpy, TMA/TPTZ systems on graphene, we used graphene supercells and sampled the Brillouin zone by a $1 \times 1 \times 1$ k-point mesh. The interaction energy $E_{\text{interaction}}$ of the TMA, TMA/Bpy, TMA/TPTZ systems with graphite is given by $E_{\text{interaction}} = E_{\text{total}}(\text{system/graphene}) - E_{\text{total}}(\text{isolated system in vacuum}) - E_{\text{total}}(\text{graphene})$.