

Supporting information

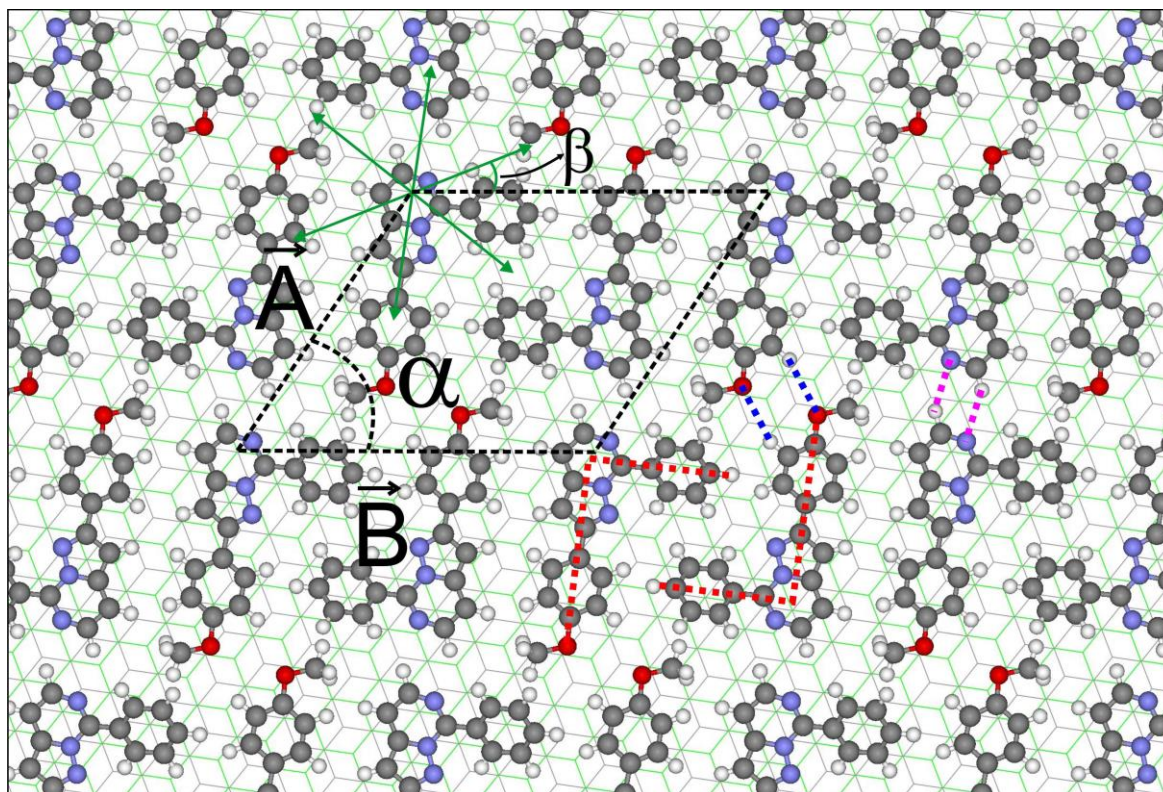


Figure S1 Force field optimized model of adlayer of **1** on bilayer graphite (Model-2). Dashed oblique marks the unit cell with the unit cell vectors \vec{A} (15.10 Å), \vec{B} (17.20 Å) and α (56.0°), the angle between them. Compared to Model-1, the relative orientation of the molecules within the assembly is different as clearly visible in α . The angle between the facets obtained in the experiments (marked by α in [Figure 5](#)), ~89°, is matching well with α obtained in Model-1. Green double-headed arrows indicate the graphite compact lattice directions. β indicates the relative orientation of \vec{B} with respect to one of the graphite compact lattice directions (21°). Magenta and blue dashed lines show weak interactions between N...H-C and O...H-C, respectively, within the assembly. Red dotted line shows the 'L'-shaped molecules. The top and bottom layers of the graphite are shown in grey and green colors, respectively.