# Self-Assembly Behavior of Alkylated Isophthalic Acids Revisited: Concentration in Control and Host-Guest Induced Phase Transformation

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## 1. Self-assembly of ISA-OC10



Figure S1: STM images and corresponding tentative models of ISA-OC10 at the phenyloctane/HOPG interface (0.5mM mM,  $V_{\text{bias}} = -0.65$  V,  $I_{\text{set}} = 0.12$  nA) showing the porous (top) and the lamellar network (bottom). (Unit cell parameters for the porous network:  $\alpha = 57.7 \pm$ 

 $1.0^{\circ}$ , a =  $3.39 \pm 0.1$  nm, b =  $3.66 \pm 0.1$  nm)

### 2. Self-assembly of ISA-OC18



Figure S2: STM image and corresponding tentative molecular model of ISA-OC18 at the phenyloctane/HOPG interface (0.47mM,  $V_{\text{bias}} = -0.85$  V,  $I_{\text{set}} = 0.2$  nA), showing the lamellar network (unit cell parameters:  $\alpha = 89.8 \pm 2.5^{\circ}$ ,  $a = 0.89 \pm 0.1$  nm,  $b = 3.82 \pm 0.2$  nm)

# 3. Large scale STM images of ISA-OC10 and ISA-OC14 at different concentrations and ISA-OC18 at submonolayer coverage



Figure S3: STM images of (a-c) ISA-OC10 and (d-f) ISA-OC14 at the phenyloctane/HOPG interface at different concentrations, showing the formation of hexameric patterns at lower concentration. a) 1.0mM,  $V_{\text{bias}} = -0.65$  V,  $I_{\text{set}} = 0.12$  nA, b) 0.49mM,  $V_{\text{bias}} = -0.65$  V,  $I_{\text{set}} = 0.12$  nA, and c) 0.1mM,  $V_{\text{bias}} = -0.65$  V,  $I_{\text{set}} = 0.12$  nA, d) 2.65mM,  $V_{\text{bias}} = -0.50$  V,  $I_{\text{set}} = 0.13$  nA, e) 1.33mM,  $V_{\text{bias}} = -0.65$  V,  $I_{\text{set}} = 0.13$  nA, and f) 0.03mM,  $V_{\text{bias}} = -0.65$  V,  $I_{\text{set}} = 0.12$  nA.).



Figure S4: STM image of ISA-OC18 at the phenyloctane/HOPG interface (0.01 mM,  $V_{\text{bias}} = -0.65$  V,  $I_{\text{set}} = 0.12$  nA). Even at sub-monolayer coverage, ISA-OC18 still uniquely forms the lamellar packing.