Supporting Information

Graphene Surface Induced Specific Self-Assembly of Poly (3-hexylthiophene) for Nanohybrid Optoelectronics: From First-principles Calculation to Experimental Characterizations

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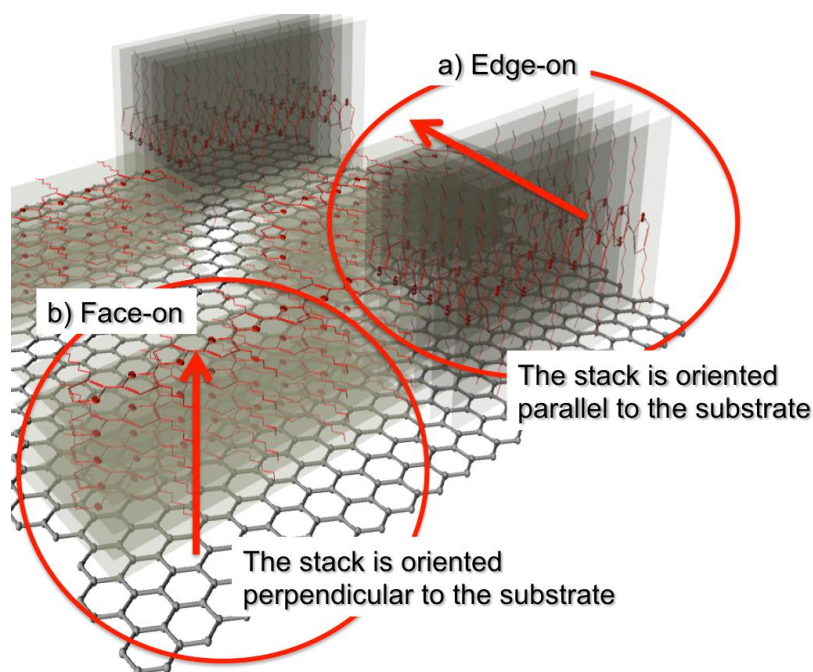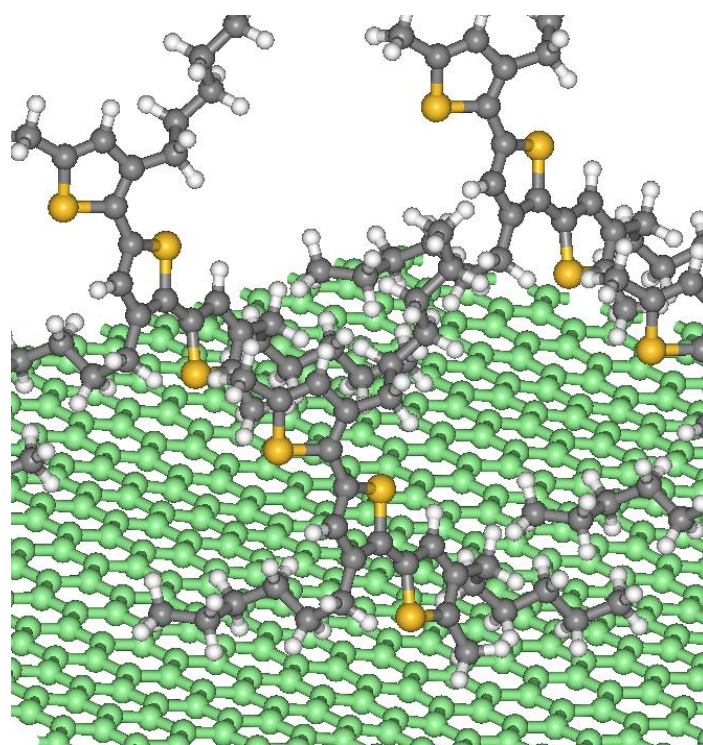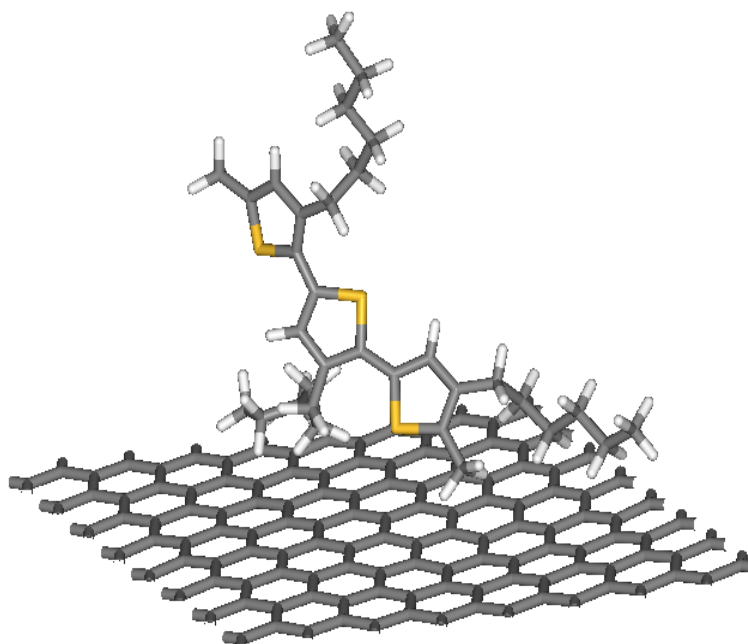*E-mail address: dchoi@khu.ac.kr (D.C.), jaeyoung88.choi@samsung.com (J.-Y.C.)*

Fig. S1. Proposed schematic models of P3HT chains on graphene monolayer.

(a)

(b)

Fig. S2. (a) Side view of Figure 1b. (b) Model of a trimer with aklyl chain reflecting the real polymer system in which the long-axis of a trimer is further oriented parallel to the graphene substrate.
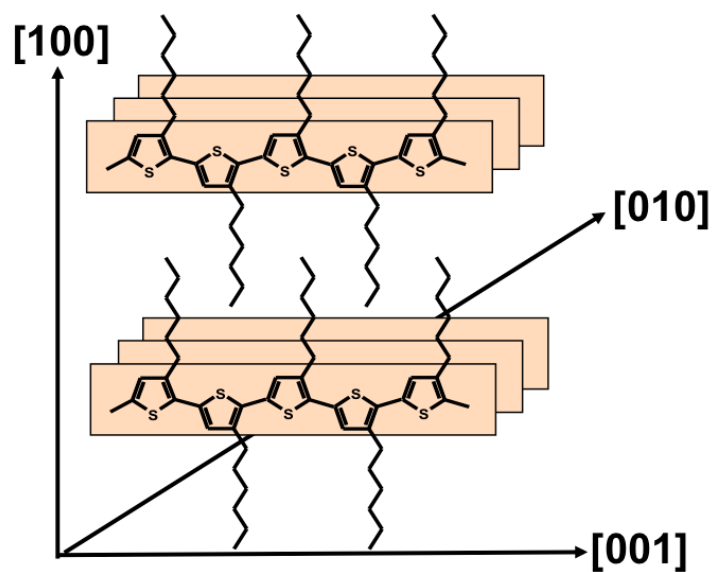
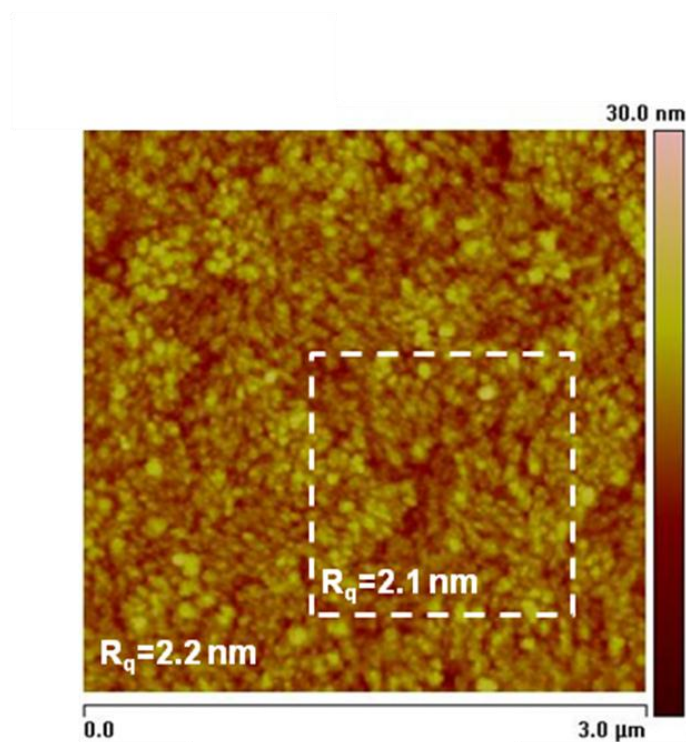**Fig. S3.** Schematic diagram of P3HT crystallography.

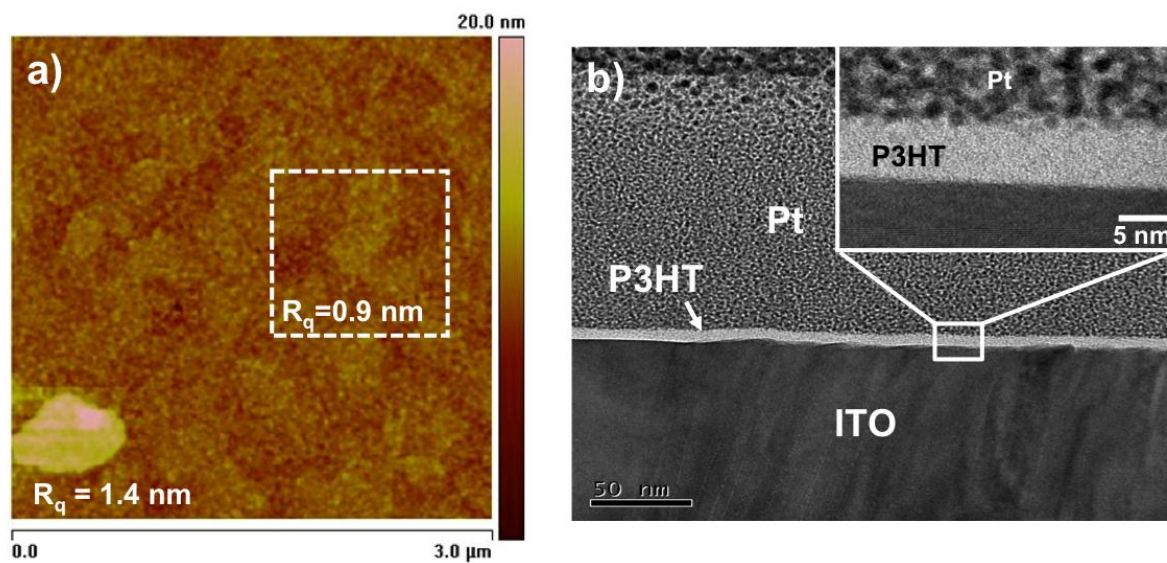**Fig. S4.** AFM image and surface roughness of an ITO substrate.

Fig. S5. Band Morphological features of a P3HT thin film spin-coated on ITO. a) AFM and b) cross-sectional TEM images.
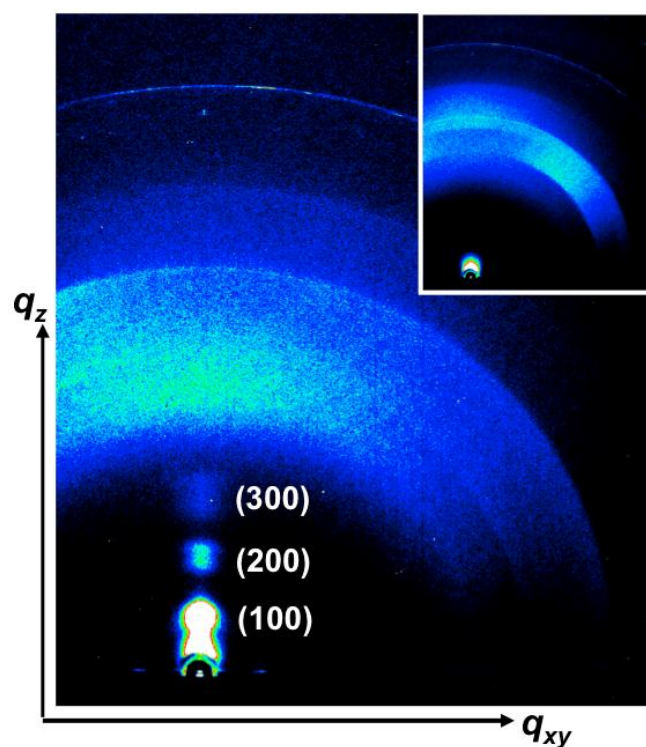

Fig. S6. 2D GIXD patterns of a P3HT film spin-coated on a ITO substrate. The inset shows GIXD pattern of ITO as a background.
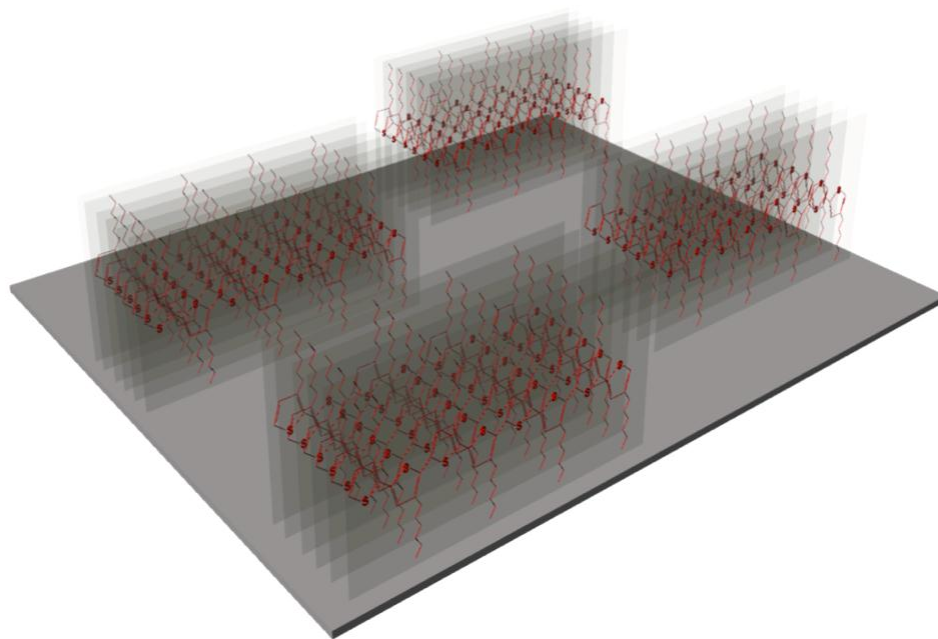
Fig. S7. Schematic illustration of arrangement of P3HT chains on an ITO surface.