Supplementary Information for

Theoretical Study of Substrate and Molecular Density Effects on Molecular Self-assembly

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Fig. S1  Self-assembled models of DPTTA molecules with number of (a) 16, (b) 20, (c) 30 and (d) 36 on Au substrate.

Fig. S2  Self-assembled models of DPTTA molecules with number of (a) 16, (b) 20, (c) 30 and (d) 36 on HOPG substrate.
Fig. S3  Snapshots of DPTTA molecules with number of (a) 16, (b) 20, (c) 30 and (d) 36 on Au substrate at 2 ns MD simulation.

Fig. S4  Snapshots of DPTTA molecules with number of (a) 16, (b) 20, (c) 30 and (d) 36 on HOPG substrate at 2 ns MD simulation.