Electronic Supplementary Material (ESI) for New Journal of Chemistry.

This journal is © The Royal Society of Chemistry and the Centre National de la Recherche Scientifique 2019

Supplementary Information for

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

Yuan Qin[a], Yingying Yang[a], Yuelin Wang[a], Xudong Wang[a], Man Yao[a,b*]

[a.] *School of Materials Science and Engineering, Dalian University of Technology, Dalian 116024, China. E-mail: yaoman@dlut.edu.cn*

[b.] *Key Laboratory of Energy Materials and Devices, Liaoning Province, China*

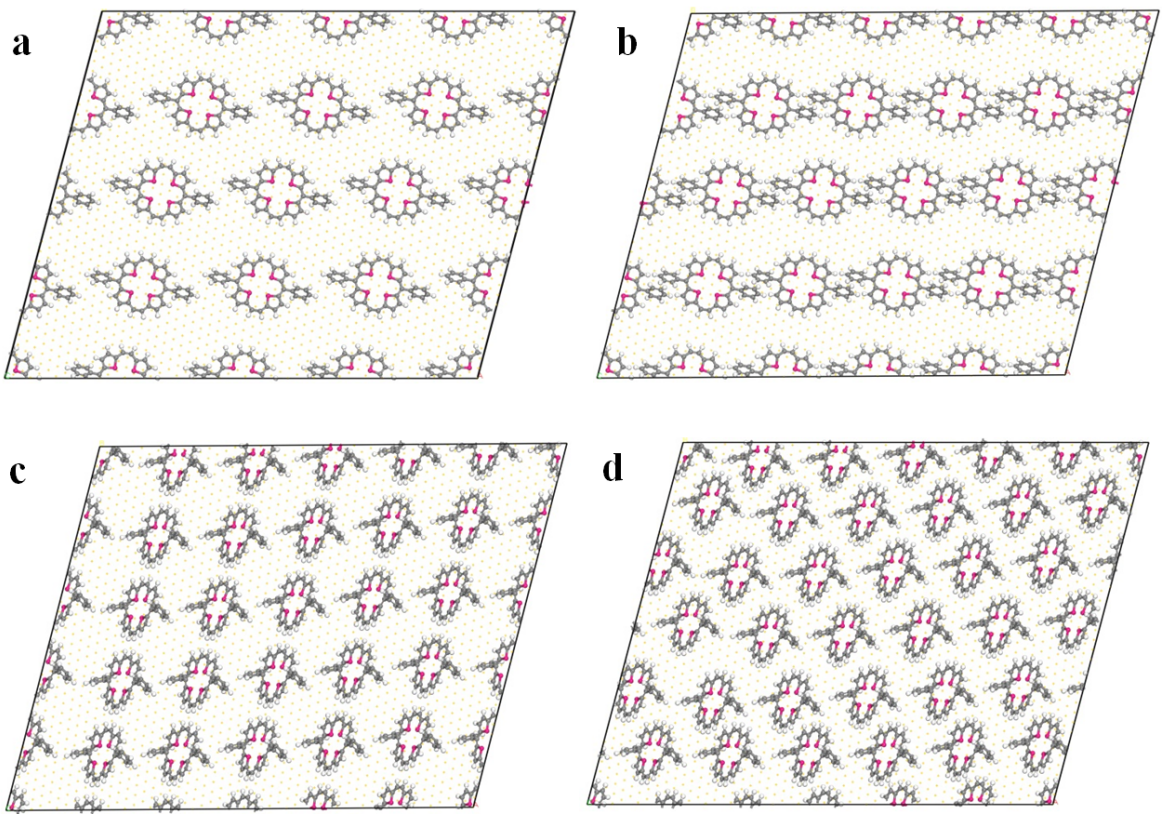

Fig. S1 Self-assembled models of DPTTA molecules with number of (a) 16, (b) 20, (c) 30 and (d) 36 on Au substrate.

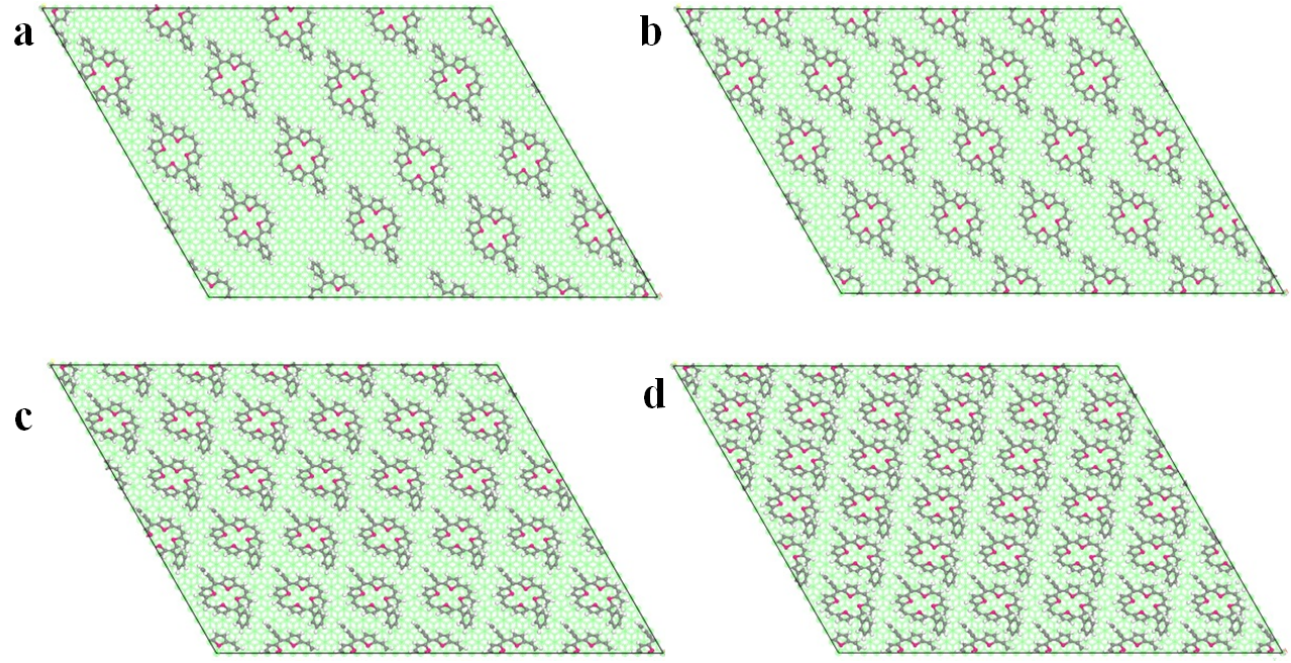

Fig. S2 Self-assembled models of DPTTA molecules with number of (a) 16, (b) 20, (c) 30 and (d) 36 on HOPG substrate.

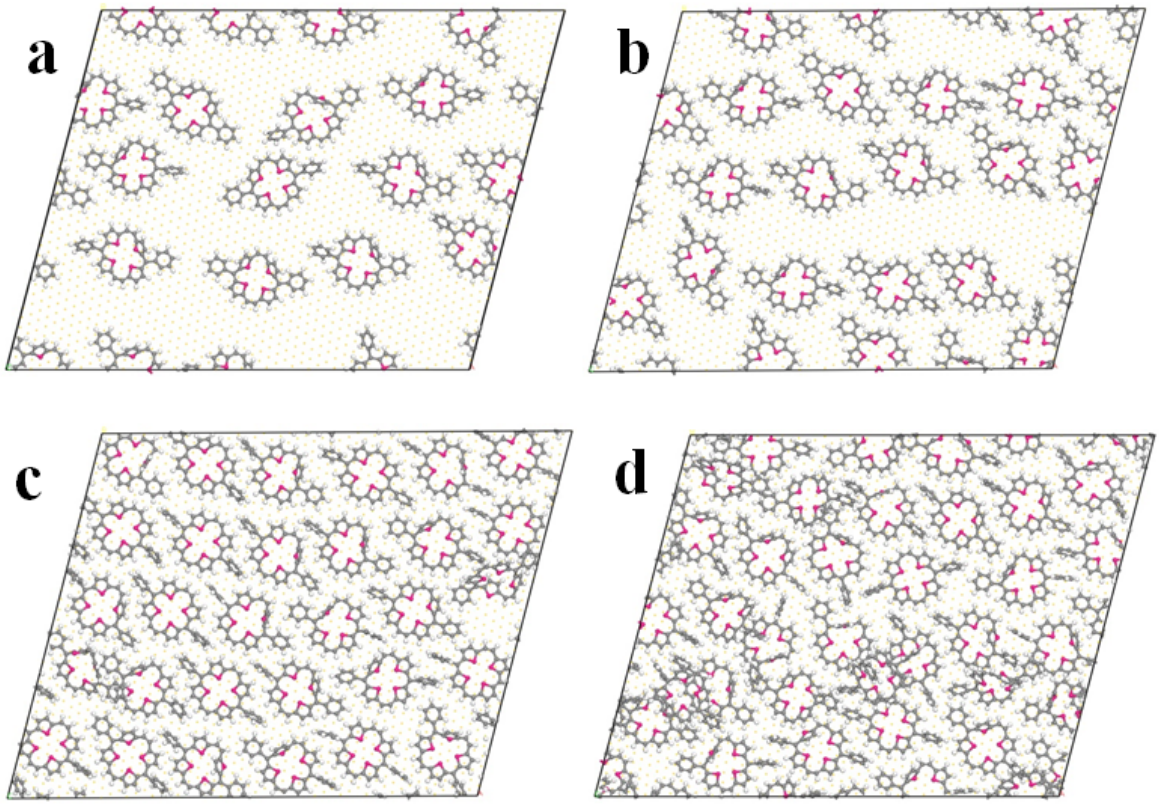

Fig. S3 Snapshots of DPTTA molecules with number of (a) 16, (b) 20, (c) 30 and (d) 36 on Au substrate at 2 ns MD simulation.

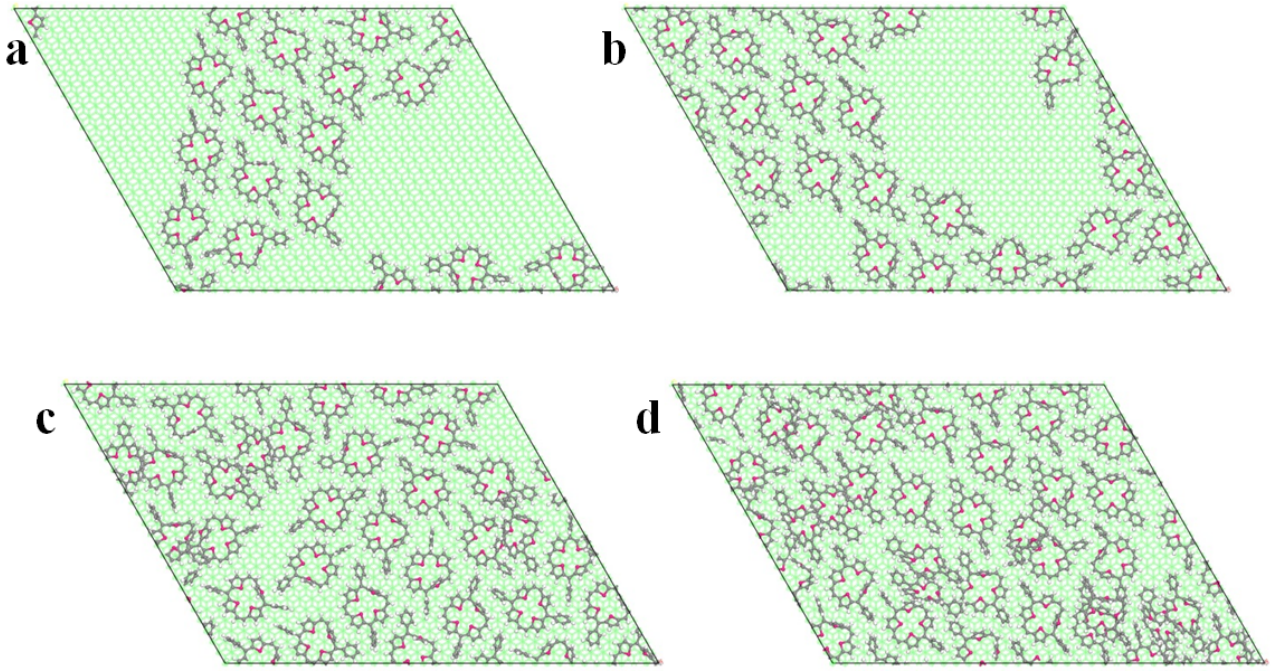

Fig. S4 Snapshots of DPTTA molecules with number of (a) 16, (b) 20, (c) 30 and (d) 36 on HOPG substrate at 2 ns MD simulation.