

Influence of Self-Assembled Monolayers on Growth and Crystallization of Rubrene Films: A Molecular Dynamics Study

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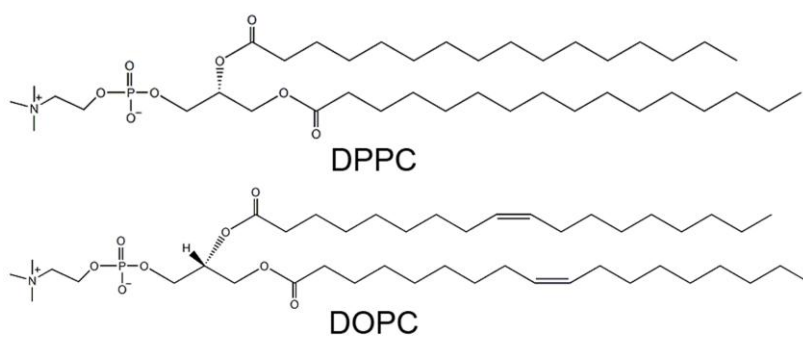


Figure S1. Schematic structure for the DPPC and DOPC molecules.

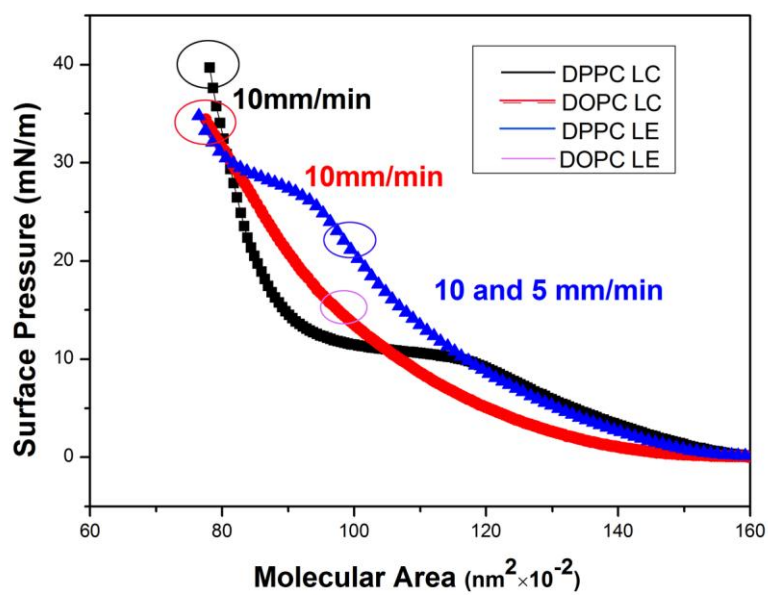


Figure S2. Experimental data for the surface pressure-molecular area isotherm of different SAMs. Colorful circle represents the molecular occupied area of single molecules of SAMs

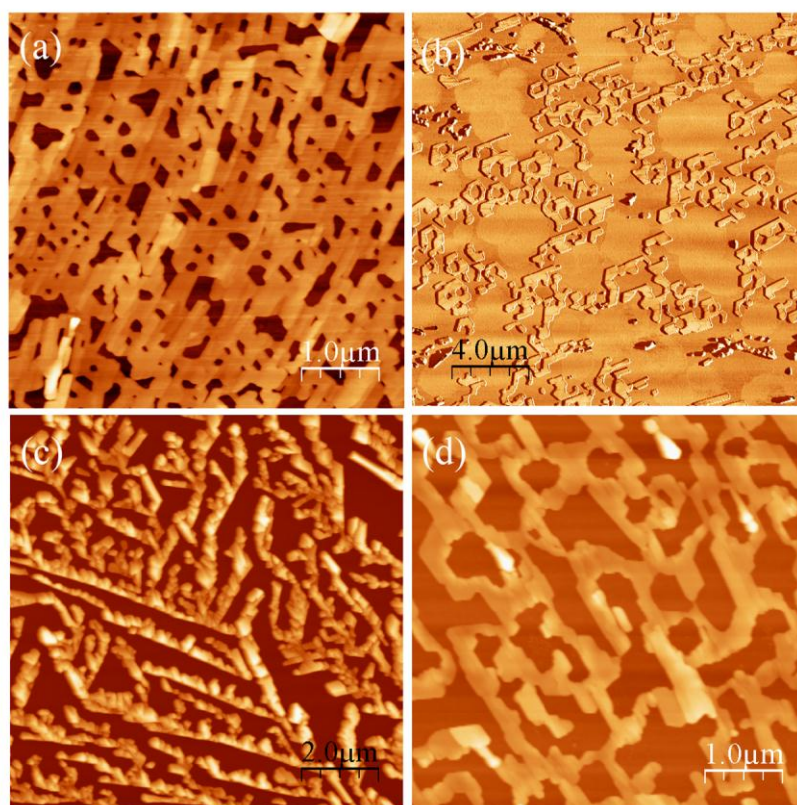


Figure S3. AFM images of rubrene thin film surfaces. (a) LC DPPC phase (B) LE DPPC phase (C) LC DOPC phase (D) LE DOPC phase

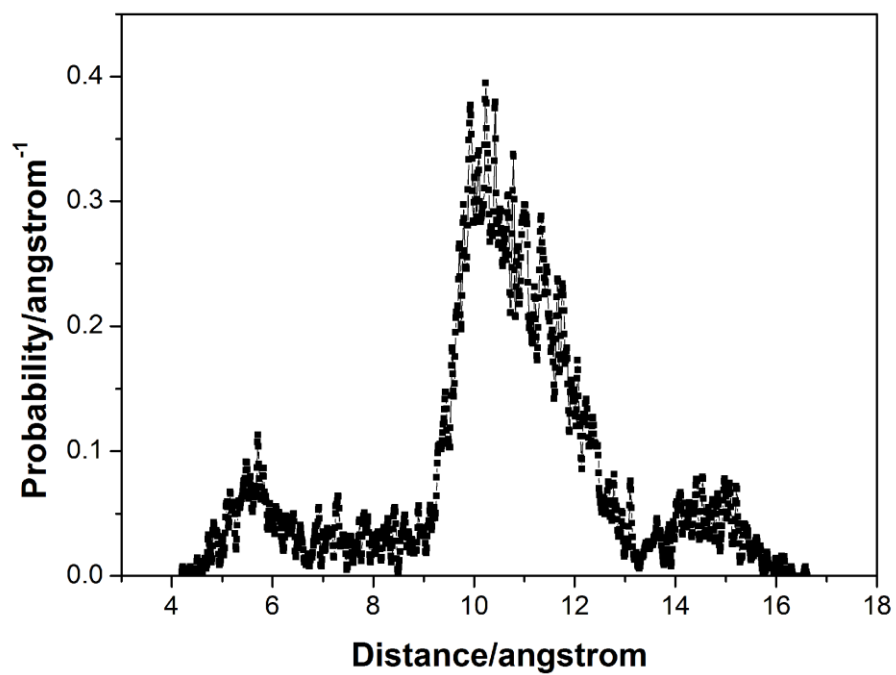


Figure S4. Probability distribution of the center to center distance of two neighboring rubrene ring pairs in LC DOPC phase.

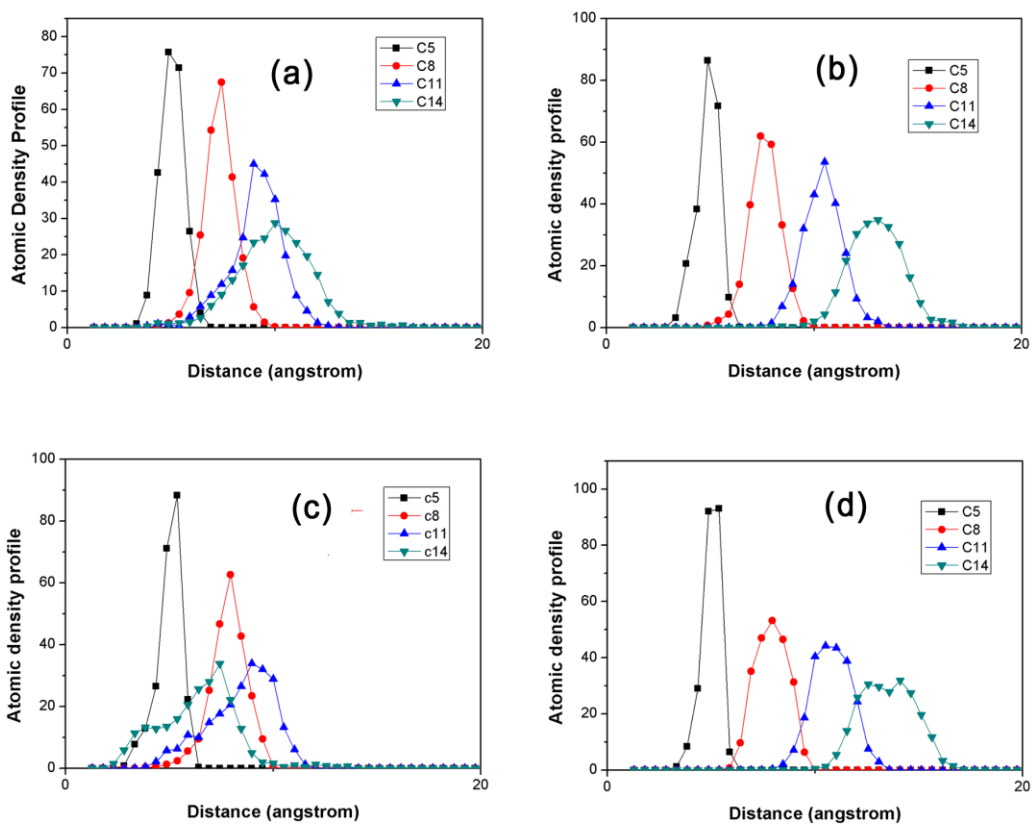


Figure S5. Atomic density profiles of C-atom of SAMs with respect to the oxide silicon surface, in the direction normal to the plane of silica surface.(ie., along the z direction) (a) LE-DPPC, (b) LC-DPPC, (c) LE-DOPC (d) LC-DOPC .

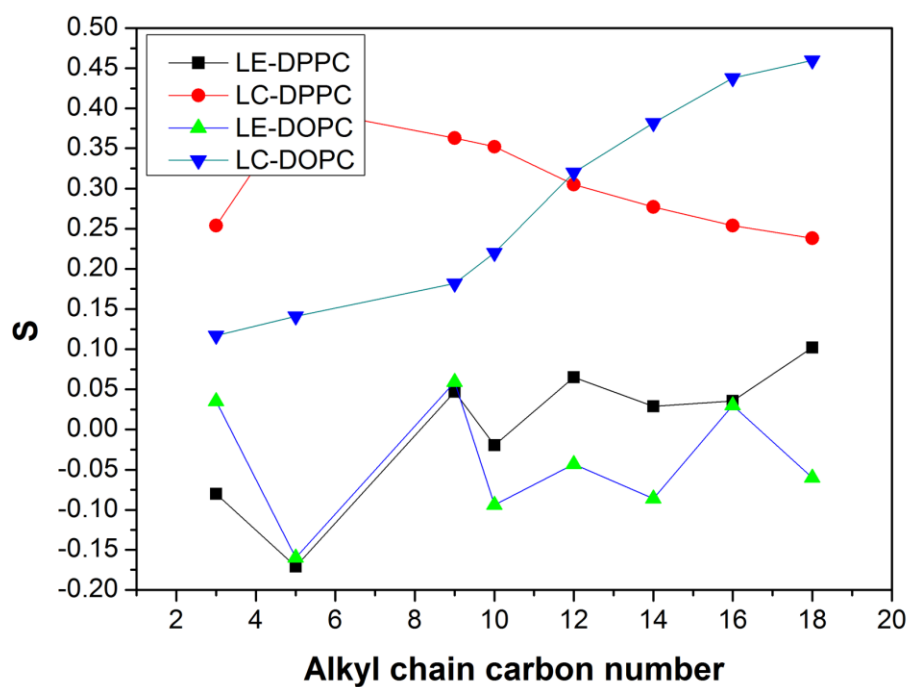


Figure S6. Order parameters S of alkyl chain at different systems.

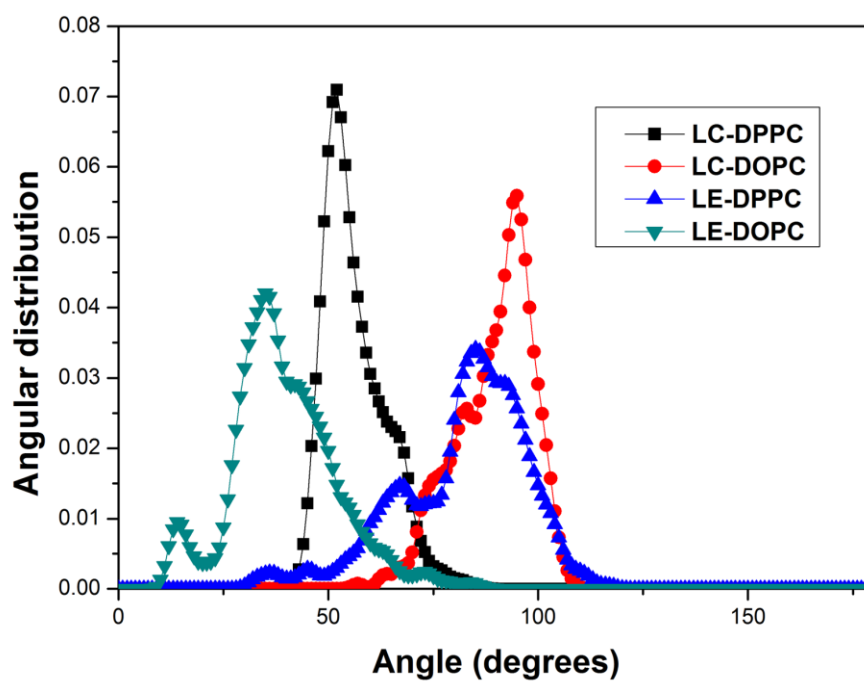


Figure S7. Angular distribution function of alkyl chains with respect to the silicon dioxide substrate at different systems.