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Supporting Information

Triangular-Shaped Molecular Random Tiling and Molecular Rotation in a Two-Dimensional Glassy Networks

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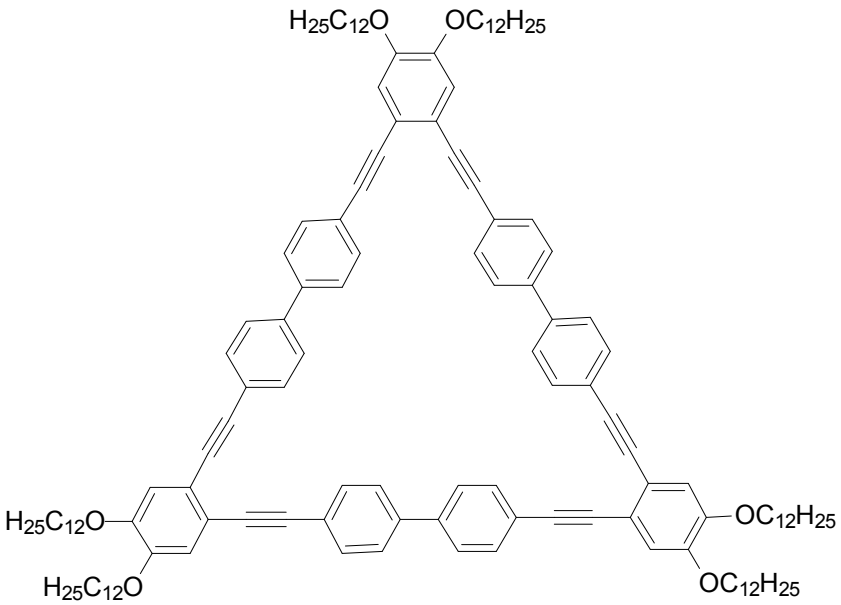
1. Experimental Section

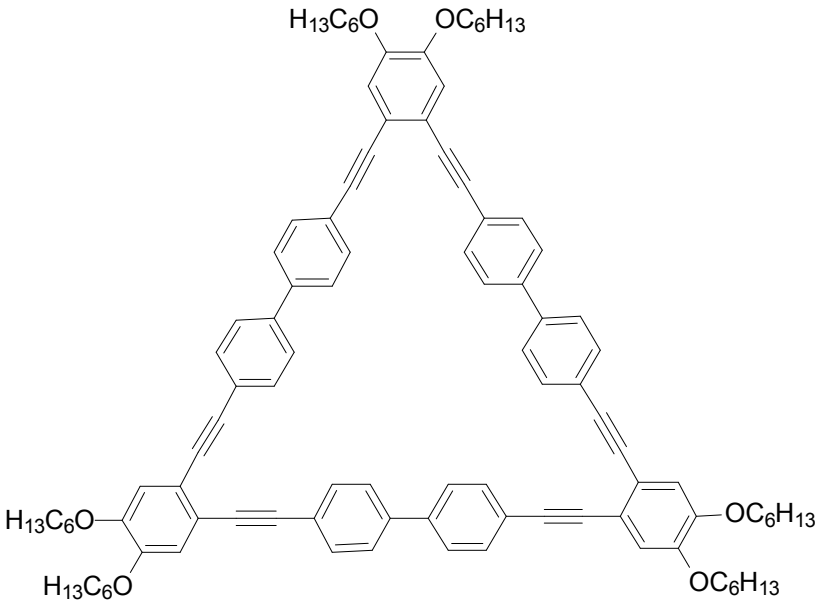
The solvents used in the experiments, 1,2,4-Trichlorobenzene (TCB) were purchased from Acros Co. and used without further purification. Macrocycle-1 was synthesized as previously reported.[1] The sample adlayer was prepared by depositing a droplet of the solution of Macrocycle on a freshly cleaved HOPG surface. All STM experiments were carried out with a Nanoscope IIIa scanning probe microscope system (Veeco Metrology, USA) at the liquid-solid interface at room temperature (21-22 °C). Tips were mechanically formed from Pt/Ir wires (80%/20%). All STM images were recorded in the constant current mode.

2. Theoretical Simulation Methods

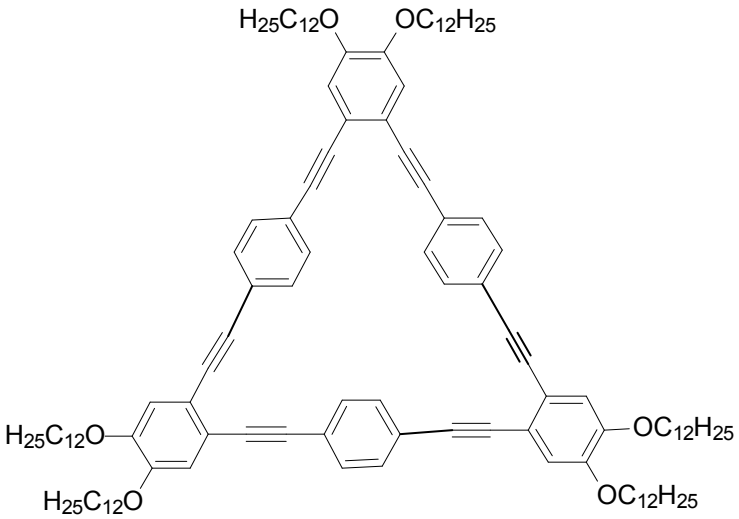
We performed periodic theoretical calculations using density functional theory (DFT) provided by the DMol3 code.[2] The Perdew and Wang parameterization[2,3] of the local exchange-correlation energy are applied in the local spin density approximation (LSDA) to describe exchange and correlation. We expand the all-electron spin-unrestricted Kohn-Sham wave functions in a local atomic orbital basis. In such double-numerical basis set polarization is described. All calculations are all-electron ones, and performed with the extra-fine mesh. Self-consistent field procedure is done with a convergence criterion of 10^{-5} a.u. on the energy and electron density.



Macrocycle-1



Macrocycle-2



Macrocycle-3

Table S1. The interaction energy between Macrocycle-1,2,3 and HOPG surface.

	Macrocycle-1	Macrocycle-2	Macrocycle-3
Interaction Energy between Macrocycle and HOPG surface	-254.97 kcal/mol	-188.37 kcal/mol	-227.13 kcal/mol

References:

[1] T. Li, K. Yue, Q. Yan, H. Huang, H. Wu, N. Zhu and D. Zhao, Soft Matter, **8,** 2405 (2012)

[2] A. D. Becke, J. Chem. Phys. **88**, 2547 (1988)
[3] J. P. Perdew and Y. Wang, Phys. Rev. B **45**, 13244 (1992)