In silico polymerization of 2D Polymers at water-surfactant monolayer interfaces

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Two-dimensional Polymers with large crystalline domains and monolayer thickness are challenging to synthesize to this day. A promising approach was introduced by Feng et al. in 2019 [1] where surfactants on a water surface were used to facilitate a 2D templating effect for the polymerization. This happens in three steps: first, spreading of the surfactants on a water surface, second, adding monomer 1 and letting it pre-assemble at the interface, and finally, adding monomer 2 which starts the polymerization. However, the exact mechanisms in each of the steps are poorly understood yet because of the dynamical behavior of the system which is difficult to characterize in experiment. Here, we use Molecular Dynamics (MD) Simulations to account for the dynamics and close the gaps between experimental observations and microscopic understanding. For this, we choose a well-known 2D Polymer synthesis route shown in Fig. 1 as model system [2]. This computational study gives valuable guidelines and insights for engineering crystalline 2D Polymers.

REFERENCES

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[2] H. Qi, H. Sahabudeen, B. Liang, M. Položij, M. Addicoat, T. Gorelik, M. Hambsch, M. Mundszinger, S. Park, B. Lotsch, S. Mannsfeld, Z. Zheng, R. Dong, T. Heine, X. Feng, U. Kaiser, Sci. Adv., 6 (2020).

FIGURES

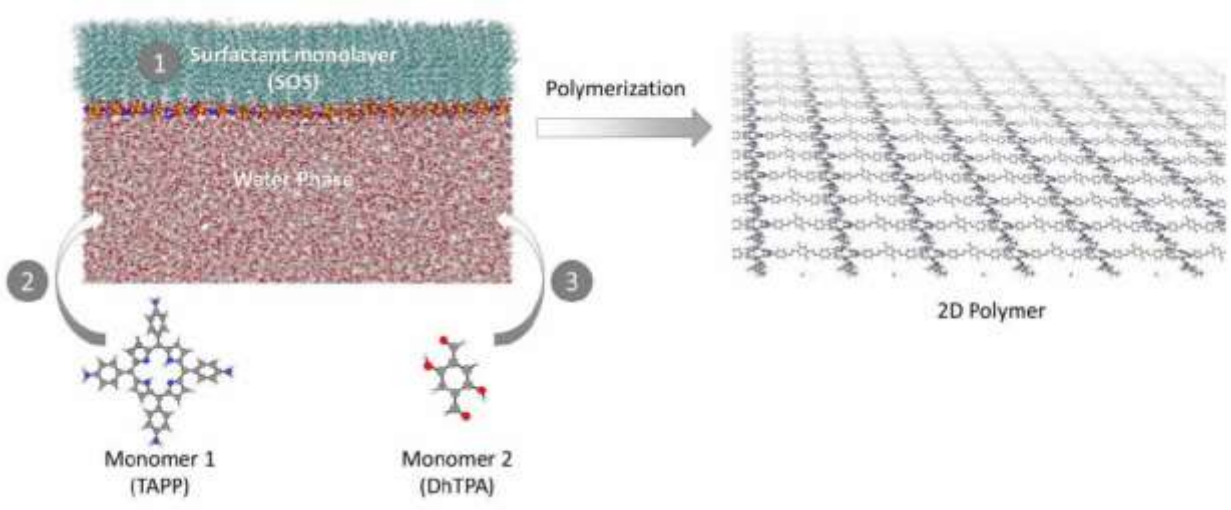

Figure 1: Steps for the polymerization at the water-surfactant monolayer interface, with sodium oleyl-sulfate (SOS) as surfactant, 5,10,15,20-tetrakis(4-aminophenyl)-21H,23H-porphyrin (TAPP) as monomer 1 and 2,5-dihydroxyterephthalaldehyde (DhTPA) as monomer 2.