

Supporting information

Molecular Dynamics Simulations of the Short-Chain Fluorocarbon Surfactant PFHxA and the Anionic Surfactant SDS at the Air/Water Interface

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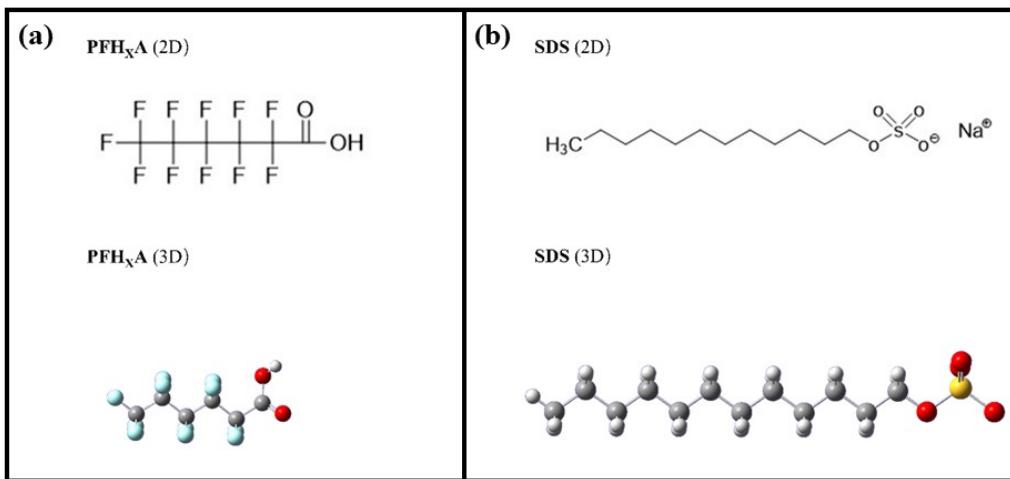


Figure S1. The 2D and 3D molecular structures of PFHxA monomer (a) and SDS monomer (b). The atomic coloring scheme is red (O atoms), grey (C atoms), yellow (S atoms), white (H atoms), blue (F atoms).

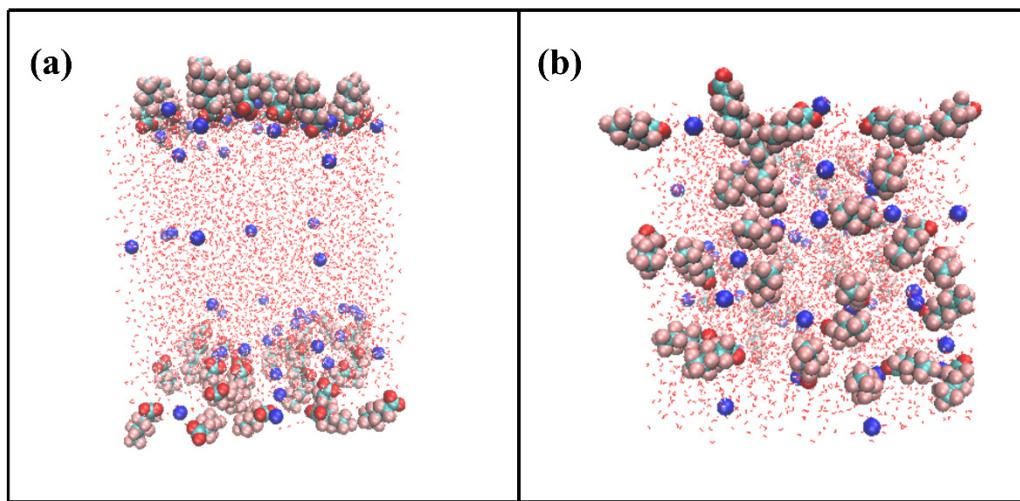


Figure S2. Side view (a) and top view (b) of the PFHxA surfactant single layer system on the gas-liquid interface..

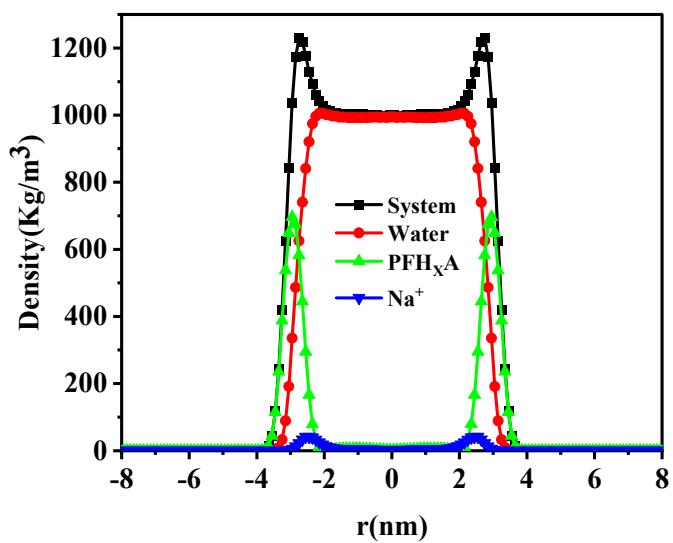


Figure S3. Density distribution profiles of pure PFHxA surfactant at gas-liquid interface.

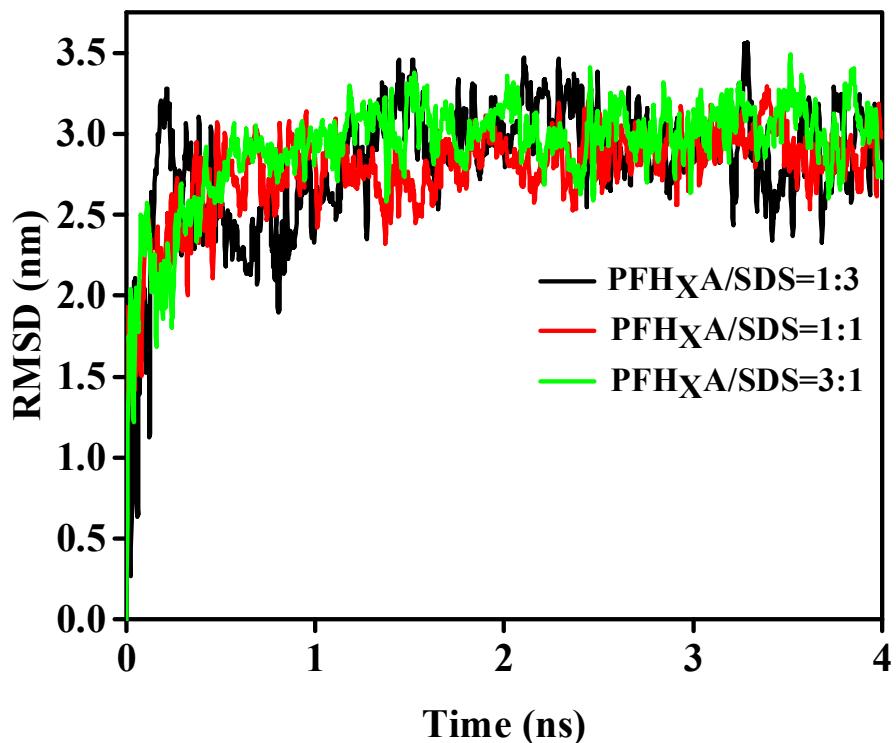


Figure S4. Average RMSD for the PFHxA surfactant in the mixed monolayers.