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Rational design and synthesis of PAH-based porous 2D thin films for membrane applications

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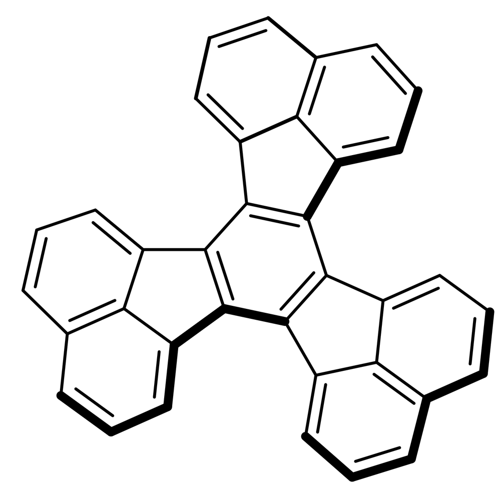
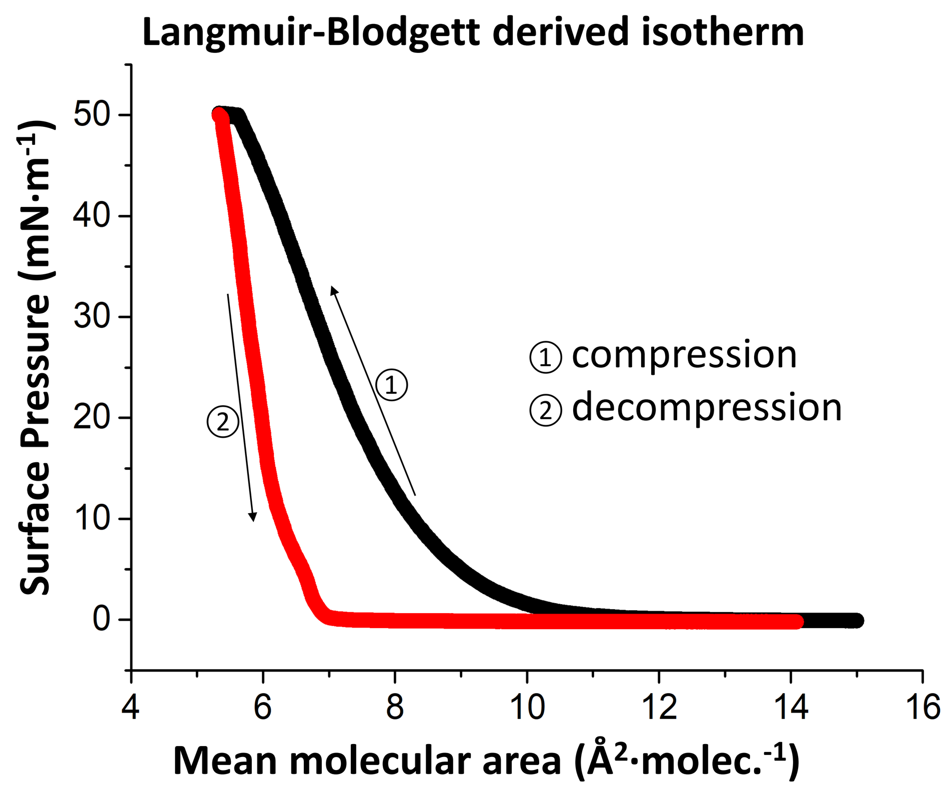
Abstract

Being able to accurately predict how polycyclic aromatic hydrocarbons (PAHs) assemble into 2D thin films *in silico* could assist in chemically designing new PAHs to integrate functionality in 2D membranes. However, *in silico* design of molecules in the context of membrane formation is still in its infancy. Instead, most *in silico* calculations have been aimed at confirming the experimental results. Experimentally, decacyclenes are found to form supramolecular 2D thin films through π-π stacking.[1] Interestingly, *in silico* predictions of decacyclenes were found to correspond with the experimental results. For the next step, we want to change the workflow around by experimentally confirming a computationally generated membrane. A successful confirmation of *in silico* predictions *via* experimental data would set the next step towards computationally predicting PAHs suitable for 2D assembly and subsequently membrane formation.



Decacyclene

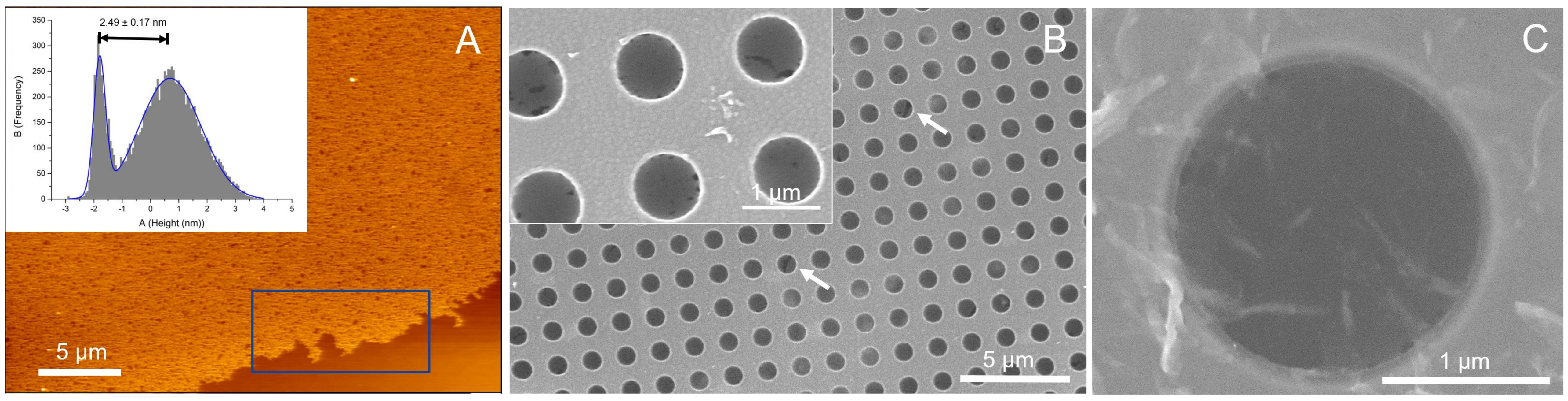
Membrane preparation



① Surface pressure increased during compression of the surface molecules.

② Hysteresis was observed during decompression, which is indicative of membrane formation.

Membrane characterization

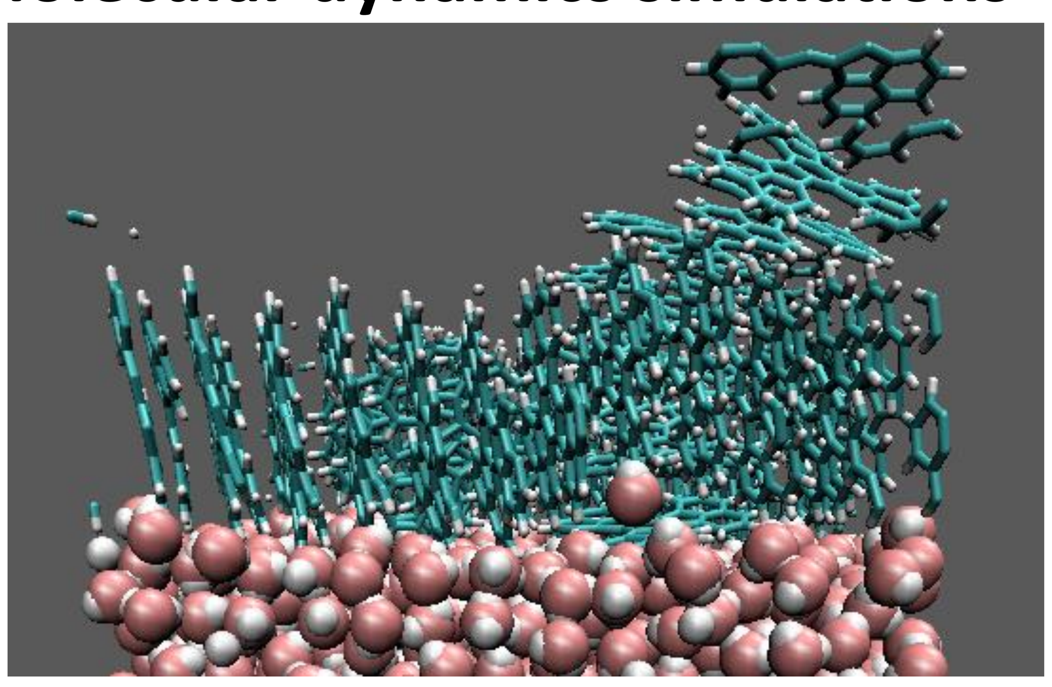


A) Atomic force microscopy (AFM) was used to measure a thickness of 2.49 ± 0.17 nm, corresponding to the width of the decacyclenes, indicating a bilayer with molecules aligned perpendicularly to the water surface.

B) Scanning force microscopy (SEM) was used to monitor the thin film with minor defects.

C) The membrane has a free-standing capability of ≥2 µm.

Molecular dynamics simulations

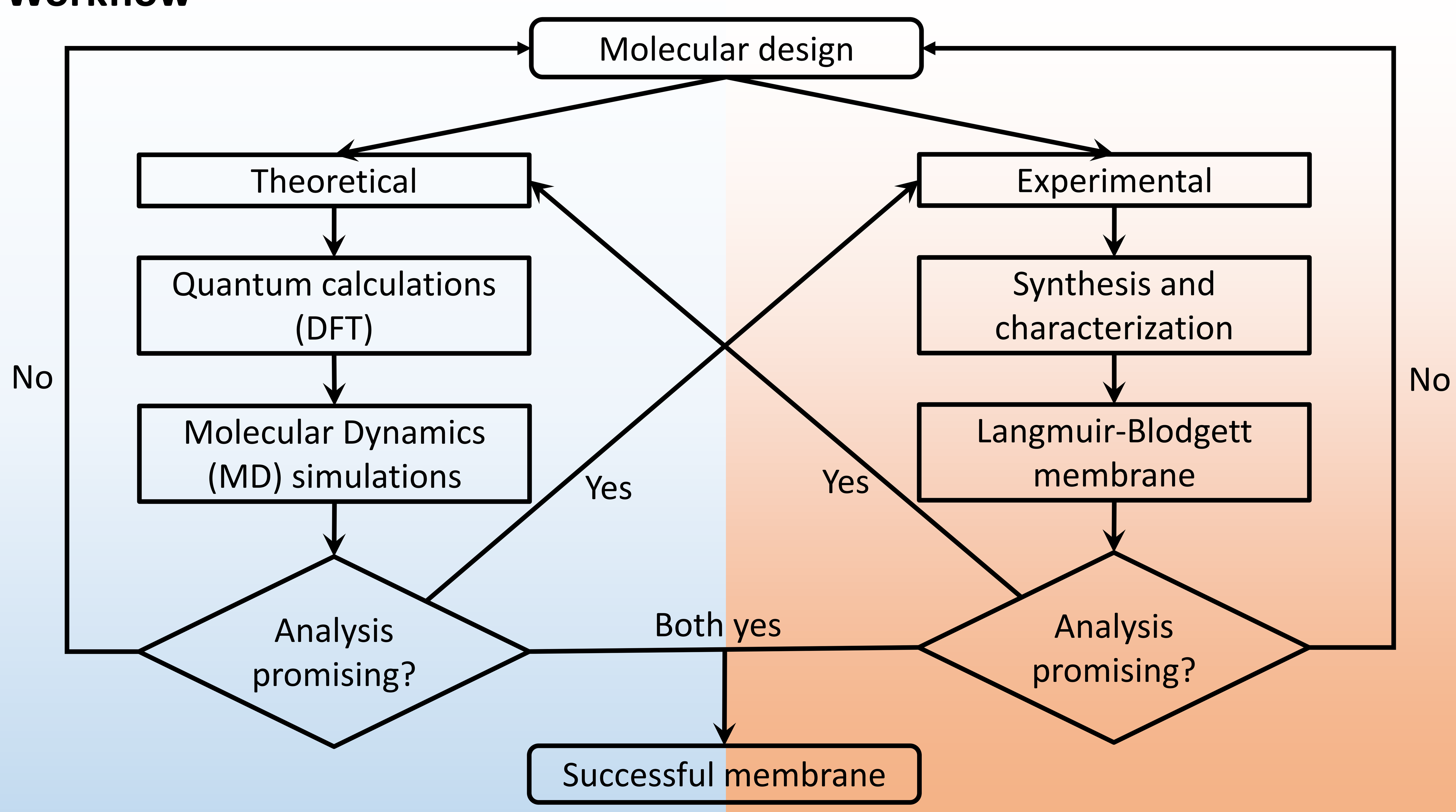


Molecular dynamics simulations (OPLS AA) of decacyclenes at room temperature and a surface pressure of 20 mN·m^{-1}.

The molecules were found to align perpendicularly to the water surface, forming intercalating rows with a so-called herringbone structure.

For more information see Dario Calvani's poster.

Workflow



Conclusion

Decacyclenes are found to form non-covalent 2D thin films both experimentally and *in silico*. Current research is aimed at computationally generating PAHs for the formation of more robust membranes and subsequently confirming the *in silico* results experimentally.

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References:

[1] A. Van der Ham et al., manuscript in preparation.

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