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

Andy Jiao, A. van der Ham, X. Liu, D. Calvani, H.S. Overkleeft, D.V. Filippov, F. Buda, and G. F. Schneider

Leiden Institute of Chemistry, Supramolecular and Biomaterials Chemistry, Leiden University, Einsteinweg 55, 2333CC Leiden, The Netherlands

a.jiao@lic.leidenuniv.nl

Accurate *in silico* prediction on how polycyclic aromatic hydrocarbons (PAHs) assemble into 2D thin films could assist in chemically designing new PAHs to integrate functionality into 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. Similarly, decacyclenes are found to form supramolecular 2D thin films through a combination of Van der Waals forces and π-π stacking both experimentally and *in silico* with corresponding results.[1] The next objective is switching the workflow around by experimentally confirming a computationally generated 2D thin film. The confirmation of *in silico* predictions with experimental data is a step further to a membrane-forming molecule generation algorithm.

References

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