Covalent Organic Framework (COF) Novel Materials for Water Cleaning

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Covalent Organic Framework (COF) membranes are novel porous membranes that can be used to filtrate water. It was proposed in previous studies that size-sieving is the main mechanism to block dye molecules. In our collaboration with Prof. Dichtel's group, we proved that actually adsorption is the main mechanism for the dye filtration. Prof. Olvera group's simulation reveals that larger dye molecules tend to cause larger entropic increase in the adsorption process, which could explain why larger molecules tend to have higher affinity. This entropic contribution is related to the depletion interaction, which is an entropic interaction with the presence of smaller molecules like water molecules. This means the solvate plays an important role in the filtration process. This finding can inspire the design of better functional membranes for water cleaning.



(A) And (B) are snapshots of simulation boxes containing COF membranes and different dye molecules. (C) and (D) are free energy graphs of adsorption process of the two dye molecules.

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