

Abstract Submitted
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Tailoring selectivity and flux in interior functionalized peptide nanotubes through self-assembly¹ SINAN KETEN, LUIS RUIZ, Northwestern University — Self-assembly of cyclic peptide nanotubes (CPNs) in polymer thin films has opened up the possibility to create separation membranes with tunable nanopores that can differentiate molecules at the sub-nanometer level. Recent studies have demonstrated that the interior chemistry of the CPNs can be tailored by inserting functional groups in the nanopore lumen (mCPNs) (Hourani et al. JACS, 2011). Through theory and multi-scale MD simulations, here we explain how the stacking ordering of binary mixtures of functional CPs can be prescribed using the entropic elasticity of conjugated polymers (Ruiz & Keten, Soft Matter, 2014). The linear self-similar coarsening growth mechanism, kinetic trapping and its effects on stacking sequences will be demonstrated (Ruiz & Keten, J. Phys. Chem. Lett., 2014). Building on these insights, we present a new approach to addressing the challenge of boosting water flux and ion selectivity simultaneously, specifically by inserting two different types of functional groups in the lumen, and by controlling CP stacking order. Simulations elucidate how functional groups inspired from biological amino acids influence the transport of water and ions through mCPNs. We find mixing functional groups to tune partial charge distributions and pore size can be used to boost flux and selectivity (Ruiz & Keten, Nanoscale, 2014). Our computational thought experiments lay the foundation for bioinspired principles to discover artificial nanochannels for separation applications.

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