Electrostatic Mechanism for Shape Selection in Chiral Molecular Assemblies

Scientific Achievement

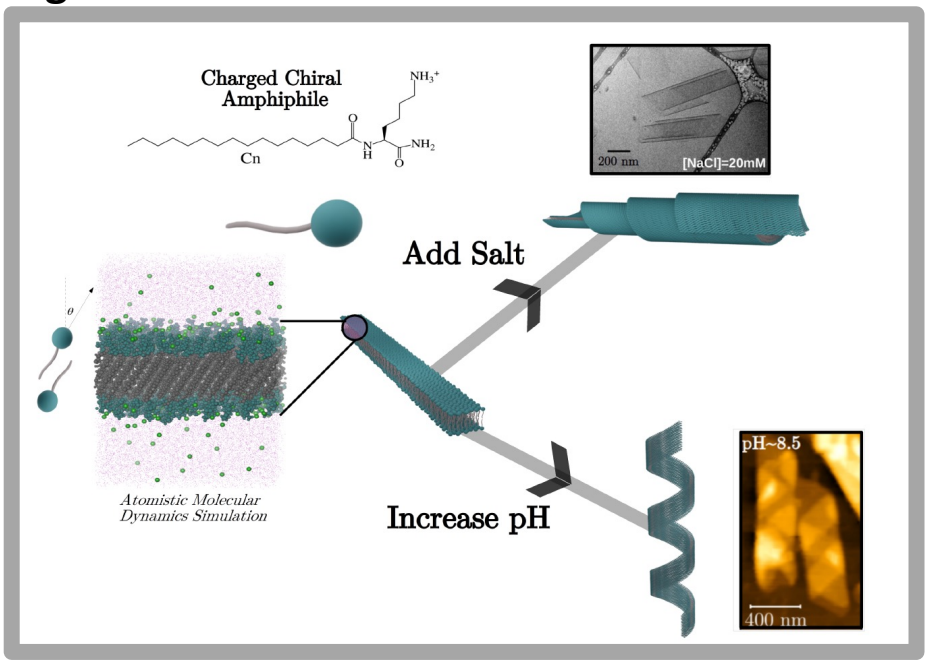
Experimental, computational, and theoretical approaches reveal different chiral molecular assemblies can be controllably created by tuning the ionic environment

Significance and Impact

Mechanism provides a rational basis for generating and controlling the nano-scale structure of membrane assemblies, enhancing the utility of molecular assemblies for biosensing, drug delivery, and nanoelectronics

Research Details

- The ionic solution environment determines whether chiral amphiphilic molecules will form a flat ribbon, helical ribbon, or scroll
- Distinct twisted membrane shapes have been previously generated in disparate molecular systems, but apriori predicting shape selection had remained challenging
- X-ray scattering measurements reveal that shape selection depends directly on the ionic solution conditions and molecular dynamics simulations show tilt ordering of the chiral molecules



Schematic of shape selection mechanism: Electrostatic interactions direct chiral shape selection. When the intermolecular electrostatic interactions of crystalline, tilted, interdigitated, chiral membranes are screened with added salt and short-ranged, scrolls are observed (cryo-TEM). In contrast, helical ribbons are observed when degree of ionization is low but electrostatic interactions are long ranged (AFM).

McCourt J.M., et al., *ACS Cent. Sci.,* (2022).

Work was performed at the Advanced Photon Source at Argonne National Laboratory

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