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Self-assembly and conjugation effects of supramolecular cyclic peptide nanotubes

L. Ruiz[1], *S. Keten[1]

[1]Department of Civil and Environmental Engineering and Mechanical Engineering, Northwestern University, Evanston, IL 60208-3111, USA

*Corresponding author: s-keten@northwestern.edu

Cyclic peptide nanotubes (CPNs) are self-assembled supramolecular systems with outstanding mechanical properties and are excellent candidates as biomimetic synthetic nanopores offering precise control of the pore diameter and the nanotube inner and outer surface chemistry.
The precise control of the self-assembly stacking sequence of CPs with different polarity can lead to the generation of nanotubes with tunable transport selectivity capabilities. We propose to use the free energy penalty associated with the polymer conjugation to direct the self-assembly of mutated CPs towards a defined stacking sequence. We present a theoretical framework and MD simulations to explain the self-assembly of conjugated-CPs. We quantify the free energy penalty induced by the polymer conjugates and we use the replica exchange method to enhance the sampling of the energy space of a coarse-grain model of the conjugated-CPs to reproduce the self-assembly stacking sequence that corresponds to the thermodynamic prediction.

Keywords: supramolecular, self-assembly, polymer conjugation, selective transport