

Multi-Scale Molecular Modeling of Fluorescent Rosette Nanotubes

Aldur Gonzales III, Takeshi Yamazaki, Belete Legesse, and Hicham Fenniri*
Department of Chemical Engineering, Northeastern University
gonzales.ar@husky.neu.edu

Background on Rosette Nanotubes (RNTs)

- Supramolecular nanomaterials formed through hydrogen bonds, a stacking, and hydrophobic effects.
- Substantial design flexibility through surface functionalization and a tunable channel for guest molecule loading.
- Applications in nanomedicine such as in coatings for medical devices, materials for tissue engineering.

Objectives

A novel triazole G-C motif was designed to self assemble into fluorescent RNTs for possible drug display and delivery. Multi-scale molecular modeling was used to predict structure, stability, and self-assembly of the RNTs.

Methods

- Model RNTs were built from the minimized G-C motifs.
- MD simulations in water, DMF, methanol, and DMSO were run from different starting configurations to determine the stability and the most probable structure of the RNTs.
- MD-RMSE was used to determine the thermodynamics, particularly, the association free energy of the RNTs.
- Hybridized MD simulations were done to predict self-assembly pathway.

RNT self-assembly and fluorescence properties in DMF (A-B) and methanol (C-D) were studied visually (A) and by TEM and fluorescence spectroscopy (B) (C-E).

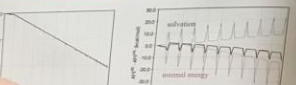
Results



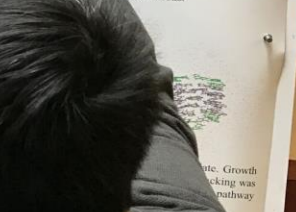
MD simulations and trajectory analysis suggest both a stable ring stack (RS) conformation (SD 3.35Å, SA -14.3°, NND 2.95Å, 7-membered rings) and a helical coil (HC) conformation (SD 3.35Å, R 4.0Å, SA 53.5°). Based on the MD studies run, the HC conformation is seen as the more favorable RNT configuration.



MD results suggest that the HC configuration of the RNT is stable in all the solvents studied. However, some motifs are seen to detach and reattach to the RNT body in DMSO, methanol, and DMF suggesting that association and dissociation is a dynamic process.



Free energy (AFE) is defined as the difference of the individual free energy of the RNT and the total free energy of the solvent. The plot shows the relative trend for both the RS (---) and HC (---) conformations. The RS conformation is more stable than the HC conformation based on the free energy landscape.



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