Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Multiscale simulations of nanoribbon structures from chromophore amphiphile self-assemblies DONGXU HUANG, ZHENWEI YAO, MONICA OLVERA, SAMUEL STUPP, Northwestern University — Finite-width self-assembled one-dimensional nanostructures have many potential applications as electronically or biologically active materials. Understanding the driving forces for supramolecular self-assembly is essential for the molecular design of new highly functional structures. Here we use multi-scale molecular dynamics simulations to study the self-assembly of chromophore amphiphiles into a nanoribbon previously shown to be useful in photocatalysis [1]. We demonstrate that the nanoribbon structure is a result of the competition between electrostatics and the hydrophobic effect. We incorporate a scaling analysis that correlates the electrostatic strength with the finite width of the ribbon. These results with additional numerical calculations show that anisotropy of the short-range intermolecular interactions and long-range electrostatics can be used to control the dimensionality of these systems. [1] Adam S. Weingarten, Roman V. Kazantsev, Liam C. Palmer, et al. & Samuel I. Stupp, Nature Chemistry, 2014

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Date submitted: 24 Nov 2015 Electronic form version 1.4