**NF Draft**

**Model and Theory (abbreviated)**

To obtain microscopic information of the protein brushes such as monomer density distributions, a polyelectrolyte continuous-space self-consistent field theory is employed. While the key process is outlined here, the details can be found in a previous work (Yokokura 2024 Biomacromolecules). In a semicanonical ensemble, the constituent proteins are modeled as charged block macromolecules immersed in a monovalent salt solution and grafted upon a non-interacting substrate.

**Results and Discussion**

*Pure brush*

SCFT-generated density distributions provide details on the morphology of the NF brushes.

Coarse-graining of filaments 🡪 number of blocks, detailed in Tables XX.

Height extracted from density distributions by 1e-05 to best approximate AFM probe touching brush

Both NFL and NFM exhibit classical brush morphologies. The mismatch in height profile for NFM may be attributed to \_\_\_. Due to the few numbers of phosphorylizable sites in both, the morphology is largely unaffected by phosphorylation.

NFH is strongly impacted by phosphorylation, where the [X, XX] segment of the protein increases in charge density significantly. This increase caused a portion of the brush to be expelled into a diffuse outer layer at low ionic strengths. As the electrostatic screening is increased, the brush morphology changes such that a condensed layer is formed at \_\_ nm, much like the flower morphologies previously predicted for NFH by SJ-SCF (Zhulina 2007 Biophysical Journal).

The height profile of NFH does not match at intermediate ionic strengths due to the pKa of the phosphate being 7.2. As the ionic strength is increased from the salt-free case, the salt ions displace the local hydrogen concentration, resulting in a lower charge fraction than used for the quenched case. At high salt concentrations, the screening effect nullifies the overestimation in charge fraction.

*NFH Del2*

Deletion of segments is straightforwardly treated by SCFT, providing physical reasoning for the trends measured experimentally.