

Abstract Submitted
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Thermodynamics, morphology, and kinetics of early-stage self-assembly of pi-conjugated oligopeptides¹ BRYCE THURSTON, Univ of Illinois - Urbana, JOHN TOVAR, Johns Hopkins University, ANDREW FERGUSON, Univ of Illinois - Urbana — Synthetic oligopeptides containing π -conjugated cores self-assemble novel materials with attractive electronic and photophysical properties. All-atom, explicit solvent molecular dynamics simulations of Asp-Phe-Ala-Gly-OPV3-Gly-Ala-Phe-Asp peptides were used to parameterize an implicit solvent model to simulate self-assembly. At low-pH conditions, peptides assemble into β -sheet-like stacks with strongly favorable monomer association free energies of $\Delta F \approx -25k_B T$. Aggregation at high-pH produces disordered aggregates destabilized by Coulombic repulsion between negatively charged Asp termini. We model simulations of hundreds of monomers as a continuous-time Markov process. We infer transition rates between different aggregate sizes and microsecond relaxation times for early-stage assembly. Our data suggests a hierarchical model of assembly in which peptides coalesce into small clusters over tens of nanoseconds followed by structural ripening and diffusion limited aggregation on longer time scales. This work provides new molecular-level understanding of early-stage assembly, and a means to study the impact of peptide chemistry upon the thermodynamics, assembly kinetics, and morphology of the supramolecular aggregates.

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