

Abstract Submitted
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Simulation and Numerical Modeling of the Self-assembly of an Optoelectronic Peptide RACHAEL MANSBACH, ANDREW FERGUSON, Univ of Illinois - Urbana — We report molecular dynamics simulations of the self-assembly of synthetic π -conjugated oligopeptides into optoelectronic nanostructures. The electronic properties provide the basis for an array of organic electronic devices, such as light-emitting diodes, field-effect transistors, and solar cells. Control of the structure, stability, and kinetics of self-assembled organic electronics by tuning monomer chemistry and environmental conditions presents a powerful route to the fabrication of biocompatible designer materials. We have performed coarse-grained simulations of the self-assembly of several hundred peptides over microsecond time scales to probe the morphology and kinetics of aggregation with molecular-level detail. We have subsequently used this simulation data to parameterize a kinetic aggregation model based on Smoluchowski coagulation theory to enable prediction of aggregation dynamics on millisecond time scales. These numerical models are now being integrated into a multi-physics model of peptide aggregation in a microfluidic flow cell developed by our experimental collaborators to model the self-assembly of diverse peptide architectures under tailored flow-fields for the fabrication of biocompatible assemblies with defined morphology and optoelectronic function.

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