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Machine learning and computation for π-conjugated oligopeptides: toward in silico design of assembled organic electronics BRYCE THURSTON, ANDREW FERGUSON, Univ of Illinois - Urbana — Self assembly of peptides has shown to be a promising approach for the fabrication of novel macromolecular materials. Oligopeptides that contain embedded π-conjugated subunits assemble to form β-sheet-like 1D ribbons with useful electronic and photophysical properties. Such aggregates have been shown to be able to produce charge separated states and to function as the active layer in an FET. Morphological and spectroscopic properties of the assembled aggregates can vary significantly with the chemistry of the peptides. We selectively study peptides having a peptide-Π-peptide architecture by employing computer simulations in order to assess the chemical dependence of such properties. We compute free energies of association, inter-peptide hydrogen bonding, and other such attributes. To speed up computation, we calculate molecular descriptors for peptides and apply machine learning techniques to produce a model to predict previously computed properties. This model performs well and lays the basis for a rapid search of chemistry space for peptides with specific attributes. This work assists in understanding the influence of peptide composition on the characteristics of aggregates, and progresses toward computationally driven design of novel bioelectronic materials.

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