The Role of Non-Covalent Interactions in the Self-Assembly of Aromatic Peptide Nanotubes

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Self-assembled peptide nanotubes have many potential applications in the fields of energy, nanobiotechnology, and nanomedicine. Peptides serve as excellent building blocks due to their high availability and versatility. Aromatic peptides tend to form dipeptides which then self-assemble into nanotubes. Currently, there is a lack of fundamental understanding as to how these nanotubes assemble. However, it is widely believed that non-covalent interactions between dipeptide units drive this self-assembly. In this study, intermolecular interactions between tryptophan-tyrosine (WY) dipeptides were investigated using various quantum-chemical computational methods. Other analyses such as natural bond orbital and energy decomposition were also applied. Several WY dimer configurations were studied for their structural, energetic, thermodynamic, and spectral properties to gain insight on the non-covalent interactions that take place between WY monomers. Our work confirms the role of π-π stacking, electrostatic, and dispersion forces in the stabilization between WY units, and likely drive aggregation of self-assembled structures from peptide-based molecular frameworks.