493c A Better Understanding of the Porphyrin Stacks: Experiments, Molecular Modeling and Simulation

Lu Yang, Huisheng Peng, Yunfeng Lu, and Hank Ashbaugh

The creation of novel supramolecular architectures through self-assembly of simple molecules is one of the most promising approaches for the design of nanodevices. Offering several attractive features for molecular self-assembly, porphyrins and their derivative have received much attention in the last two decades. Although it is believed that the major driving forces operating in the self-assembly process are the non-covalent intermolecular interactions such as pi-stacking, hydrogen bonding, and van der Waals interactions, little is know about the detailed mechanism of assembly. We present here a unique example of the formation of the ultra-large well-ordered superhelix structure based on the self-assembly of porphyrin derivative driven by these interactions. The geometry of this porphyrins derivative has been optimized using ab initio calculation to understand the structural and electronic properties. Umbrella-sampling molecular-dynamics simulations were performed to investigate porphyrin-porphyrin potentials of mean force in THF and water solution.