Hierarchical Self-Assembly of Frenkel Excitonic Nanotubes: Unraveling the Role of pH-Induced Effects

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As the climate crisis demands cleaner and more efficient energy systems, hierarchically self-assembled nanostructures are emerging as promising tools for sustainable technologies. Hierarchical supramolecular self-assembly is a crucial natural design principle that enables the formation of robust complex materials with structural order across multiple length scales. Understanding this process is essential to appreciate the mechanisms that govern molecular interactions and organization, which ultimately guide the development of novel technologies for applied science, such as solar energy conversion. Though the forces behind self-assembly (e.g. hydrophobicity) are known, the specific mechanism of how monomers form supramolecular structures remains unsolved. To address this gap, I investigated how basic pH environments affect the hierarchical self-assembly of light-harvesting nanotubes. I utilized a well-defined artificial model system: supramolecular double-walled light-harvesting nanotubes (NTs). NTs self-assemble in aqueous solution from cyanine dye molecules, which further hierarchically self-assemble into bundled single-walled NTs (b-NTs). I gradually adjusted the pH of assembly solutions to increasingly basic values (10.30, 11.10, 11.80) to elucidate its role in the self-assembly of NTs to b-NTs. My findings exhibit that a basic environment greatly accelerates this bundling process. B-NT formation normally takes weeks to months, but in a basic environment this process took only 24 hours. By revealing how small pH shifts can drastically affect nanoscale organization, my results demonstrate the immense potential of environmental parameters in developing strategies that utilize this controllable molecular self-assembly process to produce well-designed nanostructures.

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