

Experiment-Inspired Computational Chemistry of Polydiacetylene Supramolecular Assemblies

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Responsive polymers, undergoing changes in light absorption and emission properties in response to stimuli, have been extensively investigated as key smart materials. Among the responsive polymer materials investigated, polydiacetylenes (PDAs) have gained special attention owing to their unique optical properties well-known for a blue-to-red transition. Despite prolific empirical efforts to date for developing stimuli-responsive PDA-based materials and devices, a few reports described mechanisms on blue-to-red colorimetric transition, all of which are molecular conformational arguments that are rather conjectures and remain unproved. Herein, we adopted an “experiment-inspired” theoretical quantification with multiscale molecular dynamic simulations and quantum mechanical computations, by mimicking entire experimental procedures. In this presentation, we present theoretical investigation of PDAs revealing mechanisms of their assembly, polymerization and colorimetric transition.