

Subcomponent self-assembly is a synthetic methodology that utilizes covalent and coordinative bonds to create complex three-dimensional supramolecular architectures. This approach involves the use of simple organic building blocks and metals to construct extensive metallosupramolecular structures. By leveraging dynamic covalent reactions, this strategy provides a built-in error-checking and correcting mechanism, making it advantageous over classical synthesis methods. Notable architectures that have been successfully constructed using self-assembly include helicates, mechanically interlocked molecules, and functional capsules.

Metal-organic molecular cages are three-dimensional molecules with well-defined internal cavities. They have gained attention not only for their unique structures but also for their remarkable properties and functions. Metal-organic capsules have demonstrated various intriguing features, leading to their application in diverse fields. They have been used for separating small molecules, sensing, generating metal nanoparticles, drug delivery, anion transport, and performing challenging catalytic transformations under typical reaction conditions. The tailored voids of molecular capsules provide a protected environment for trapping reactive species and allow for selective incorporation and release of molecular cargo through intramolecular interactions with the host. Overall, the design and utilization of metal-organic capsules hold great potential for advancing supramolecular chemistry and its practical applications.

The primary objective of this research project is to develop a novel variant of self-assembly, known as tautomerism-coupled subcomponent self-assembly, for the creation of molecular cages with exciting functions. These cages will have adaptable cavities that can be modified to suit the requirements of guest molecules. The project aims to explore the interconvertibility and dynamics of supramolecular complexes to develop multifunctional, stimuli-responsive capsules with applications in various fields, including guest binding, protection, transformations, extraction, ion transport, and metal cluster stabilization.

The project focuses on the exploration of iminopyrroles, a class of compounds that bear a structural resemblance to iminopyridines but offer unique features. While iminopyridines have been extensively studied in self-assembly, iminopyrroles remain relatively unexplored. The subtle structural difference between the two compounds allows iminopyrroles to exhibit different coordination preferences and undergo metal-mediated tautomerization. These properties make iminopyrroles promising candidates for the design and synthesis of molecular cages with adaptable cavities and stimuli-responsive properties. The project's significance lies in the potential impact on diverse areas such as atomically precise nanoclusters, heterogeneous catalysis, and luminescent materials.

The successful completion of this research project will result in the development of a new variant of self-assembly, tautomerism-coupled subcomponent self-assembly, for the synthesis of pyrrole-based molecular cages with stimuli-responsive functions. These cages will have adaptable cavities and demonstrate intriguing features such as guest binding, protection, transformations, extraction, ion transport, and metal cluster stabilization. The project aims to contribute to understanding supramolecular chemistry and have potential applications in various fields, including materials science, catalysis, and drug delivery.