PolyMOCs (polymer-linked metal-organic cage) represent a cutting-edge intersection of supramolecular chemistry and materials science. Incorporating MOCs into gel matrices has opened up new possibilities for developing advanced materials with tunable mechanical properties, catalytic activities, and molecular encapsulation capabilities, unattainable in conventional gels or metal-organic frameworks. The inclusion of MOCs in gels enhances the mechanical strength, porosity, reactivity, and functional properties of composite materials. Reversible coordination bonds in MOCs enable dynamic behavior within the gel, such as self-healing, responsiveness to external stimuli, and controlled release of encapsulated molecules. Such dynamic properties are particularly advantageous for drug delivery applications, where precise release profiles are essential. The field of hybrid supramolecular gels containing MOCs is a rapidly growing area of research with significant potential for creating next-generation functional materials. By combining the dynamic and reversible nature of supramolecular interactions with the structural and functional versatility of MOCs, scientists are paving the way for new materials adaptable to a wide range of applications, from biomedicine to environmental remediation. Continued research and innovation in this field are crucial for overcoming current challenges and unlocking the full potential of these hybrid materials.

The objective of this project is to develop a new class of dual-porosity materials utilizing metal-organic cages (MOCs) embedded in gel matrices that autonomously adjust their properties. The primary goal is to control host-guest interactions in two types of pores: MOC micropores and gel mesopores, enhancing both structural adaptability and catalytic potential. This research has the potential to uncover previously unknown mechanisms of host-guest control and responsiveness to stimuli, advancing knowledge of supramolecular dynamics and opening new perspectives in sustainable catalysis, chemical separation, and smart materials. The research hypothesis proposes that leveraging the encapsulation properties of nested MOCs within the gel will achieve greater control and improved material performance in supramolecular polymer networks compared to traditional materials. PolyMOC gels, which form hollow metal-organic cages with host-guest binding sites within their cavities, will serve as an ideal model to validate this hypothesis. Their distinctive structure will demonstrate how nested interactions can significantly influence material properties in ways unattainable with traditional designs. To verify this hypothesis and achieve the desired results, the project adopts a research model combining two distinct reversible coordination bonds (imine-based and β-diketone-based) with nested host-guest interactions within MOC cavities. The building blocks are designed to produce a wide range of MOCs with varying pore sizes and geometries, allowing for adaptation to diverse guest molecules. β-Diketone units, known for their strong affinity for divalent and trivalent metals, have been selected as a key driving force for incorporating MOCs into polymer gels, forming stable yet reversible complexes. This approach provides a systematic pathway for controlling material properties and promoting innovation in supramolecular chemistry.

The project addresses significant challenges in materials science, particularly in integrating orthogonal, reversible coordination bonds with nested host-guest interactions, which remain largely unexplored. The project aims to capitalize on the intrinsic properties of MOCs to create materials with improved performance metrics. Understanding these mechanisms is crucial for achieving encapsulation, separation, and catalytic activity that could mimic or even surpass the efficiency of known synthetic materials and natural enzymatic systems. This is a novel approach, as existing studies have not fully explored the synergistic effects of integrating MOCs into gel matrices. The outcomes of this research will include: (I) efficient and selective systems for separation and purification, and (II) new, high-performance catalytic systems.