PEPTIDE SELF ASSEMBLY CONFERENCE 2026
MAINZ. GERMANY
FROM DYNAMIC STRUCTURES TO FUNCTIONAL MATERIALS

Single Amino Acid and Minimalistic Peptide Self-Assembly as a Platform for Functional Soft Materials

Ipsita Sahu, Priyadarshi Chakraborty*
Department of Chemistry, Indian Institute of Technology Hyderabad, Sangareddy, Telangana, 502284
E-mail id: cy23resch01002@iith.ac.in, priyadarshi@chy.iith.ac.in

Abstract: Nature employs molecular self-assembly to create complex functional systems from simple building blocks.[1] Inspired by this principle, we explore how amino acid and minimalistic peptide derivatives can be engineered into multifunctional supramolecular materials. The strategic introduction of two Fmoc groups into the α- and ε-amino positions of lysine in the dipeptide Fmoc-Lys(Fmoc)-Phe significantly enhances aromatic interactions and hydrophobicity, yielding a supergelator with a critical gelation concentration (0.05% w/v).[2] The resulting hydrogel exhibits remarkable self-sustaining and self-healing behavior, driven by dynamic supramolecular interactions within its nanofibrous networks. Nanoengineering these assemblies with edge-functionalized graphene oxide yields conductive soft matter with enhanced mechanical stability and efficient charge-transport properties, expanding their potential for sensing and bioelectronic applications.[2] In parallel, the single amino acid derivative (Fmoc-Trp) provides a minimalistic platform for investigating the emergence of catalytic function through molecular self-assembly.[3] The confined, highly organized microenvironment of the nanofibrous matrix promotes enzyme-like catalytic activity, and the integration of graphene-based nanomaterials further augments catalytic performance.[3] Fmoc-Trp gel also serves as a versatile nanoreactor for the in-situ generation and stabilization of metallic nanoparticles without external reducing or capping agents, yielding hybrid materials with diverse catalytic functions, including peroxidase-like activity, catalytic degradation of pollutants. To enhance processability and practical utility, the supramolecular hydrogels were engineered into reusable core-shell bead architectures that integrate synthetic and biomimetic catalysis within a single platform. The nanoparticle-loaded bead systems facilitate efficient C-C bond-forming transformations under mild conditions, including challenging reactions involving sulfur-containing substrates, while exhibiting remarkable resistance to deactivation by Lewis basic amines and excellent recyclability over multiple cycles. Collectively, these findings underscore the ability of amino acid and minimalistic peptide self-assembly to translate molecular design into emergent material functions.

References

1. G.M. Whitesides, B. Grzybowski, *Science*. **295 ,** 2418-2421 (2002).
2. I. Sahu, Y. Tang, Z. Wang, S. Naskar, T. Vijayakanth, V. V. Adole, G. Wei, P. Chakraborty, *J. Mater. Chem. A.* **12**, 4169-4183 (2024).
3. I. Sahu, D. Saha, S. Pande, S., J. Verma, P. Chakraborty, *ACS Appl. Mater. Interfaces*, **17**, 48240-48256 (2025).