

Catalytic Amplification and Regulation within Intra- and Intermolecular Cavities

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Molecular cavities, or pockets, provide unique microenvironments that enzymes use to encapsulate substrates and drive selective chemical transformations. Inspired by this concept, our group explores synthetic compounds and materials that feature similar confined spaces to mimic enzymatic catalysis. We focus on intramolecular cavities inherent to macrocyclic molecules and interligand voids that emerge during the self-assembly of organothiols on nanogold surfaces (Figure 1). In this presentation, I will discuss how these artificial systems enable catalytic amplification [1,2] and inhibition [3,4], selective product formation [4,5] and reaction control [4-7] revealing key parallels with natural enzymes.

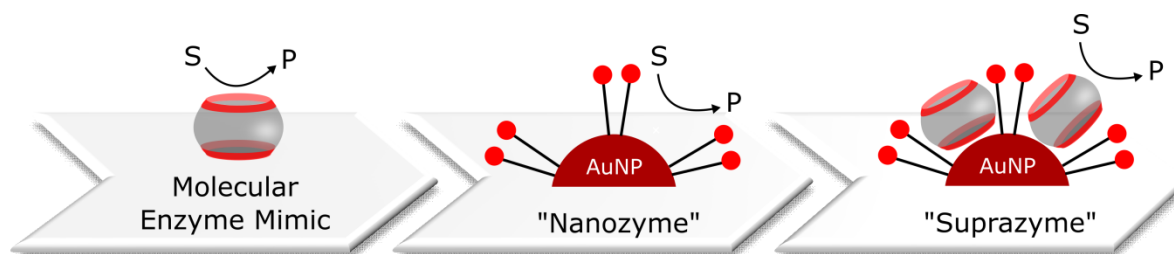


Figure 1: Evolution of enzyme mimics through increasing complexity

References:

- [1] P. Hyziuk, M. Flaibani, P. Posocco, V. Sashuk, *Chem. Sci.* **2024**, 15, 16480-16484.
- [2] V. Sashuk, H. Butkiewicz, M. Fiałkowski, O. Danylyuk, *Chem. Commun.* **2016**, 52, 4191-4194.
- [3] N. Rad, V. Sashuk, *Chem. Commun.* **2022**, 58, 5249-5252.
- [4] N. Rad, O. Danylyuk, V. Sashuk, *Angew. Chem. Int. Ed.* **2019**, 58, 11340-11343.
- [5] N. Rad, V. Sashuk, *Chem. Sci.* **2022**, 13, 12440-12444.
- [6] M. Kravets, M. Flaibani, M. Szewczyk, P. Posocco, V. Sashuk, *ACS Catal.* **2023**, 13, 15967-15976.
- [7] M. Szewczyk, G. Sobczak, V. Sashuk, *ACS Catal.* **2018**, 8, 2810-2814.