

Diastereoselectivity in low-symmetry metal-organic cages

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Metal-organic cages (MOCs) are host architectures of interest for applications in catalysis, sensing and stabilisation of reactive species, amongst others. The vast majority of MOCs reported are highly symmetrical to facilitate the self-assembly process. Molecular recognition of anisotropic substrates, however, would be greatly enhanced with lower symmetry MOCs. The significant challenge in the synthesis of low-symmetry MOCs is ensuring high fidelity in the self-assembly process to avoid forming a library of isomeric hosts.

We have been interested in developing design strategies to bias the formation of particular MOC isomers from unsymmetrical ligand scaffolds. Towards this, we have successfully used covalent tethering as well as geometric and coordination-sphere design parameters to induce diastereoselective assembly of palladium(II)-based MOCs from ligands lacking bilateral symmetry. We have also begun to develop high-throughput computational methodologies to aid in the design of such systems, reducing costly trial-and-error synthetic discovery through effective computational forecasting of self-assembly outcomes.