

Metallosupramoleculer Architectures of Bile Acid Derivatives: from Metallosupramolecular Cages to Infinite Coordination Particles

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Bile acids (BAs) are enantiomerically pure steroid compounds synthesized in human liver from cholesterol. They participate in enterohepatic circulation in digestion of lipids and lipophilic nutrients. BAs differ from each other by number and spatial orientation of hydroxyl groups located in the steroid skeleton and contain one carboxylic acid group attached to the steroid skeleton through an alkyl chain. These groups can be chemically modified into various coordination sites with a control over the bend angle, topicity, and flexibility of the final ligand. We have shown that coordination-driven self-assembly of these BA-based building units can lead to many metallosupramolecular structures (MSS) by varying reaction conditions, *i.e.*, solvent, metal salts, or metal-to-ligand ratio. Owing to the properties of the BAs, these MSS could be promising candidates for diverse applications, from basic host-guest chemistry, recognition to biomedical applications. Despite of these facts, BA-based coordination metallosupramolecular structures were unexplored until recently (Figure 1a).^{1,2}

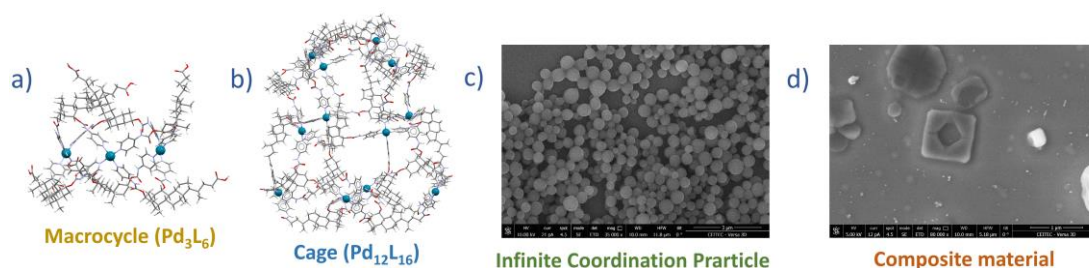


Figure 1. BA-based metallosupramolecular architectures.

Inspired by the discovery, we have designed and synthesized BA-based Pd₆L₈ and first-ever Pd₁₂L₁₆ metallosupramolecular cages (Figure 1b) using tritopic pyridyl ligand and square planar Pd²⁺ *via* molecular paneling method. Pyridyl coordinating ligands and Pd²⁺ salts are the most explored combination in metallosupramolecular chemistry. Therefore, design and synthesis of the next generation of BA-based non-pyridyl biocompatible ligands were performed. These novel ligands upon coordination with various metal salts form infinite coordination particles³ and composite materials (Figure 1c, Figure 1d). In my presentation I will describe the basic principles, synthesis, and structural details of these metallosupramolecular architectures which provide insight into self-assembly of unsymmetric natural molecule-based ligands.

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