

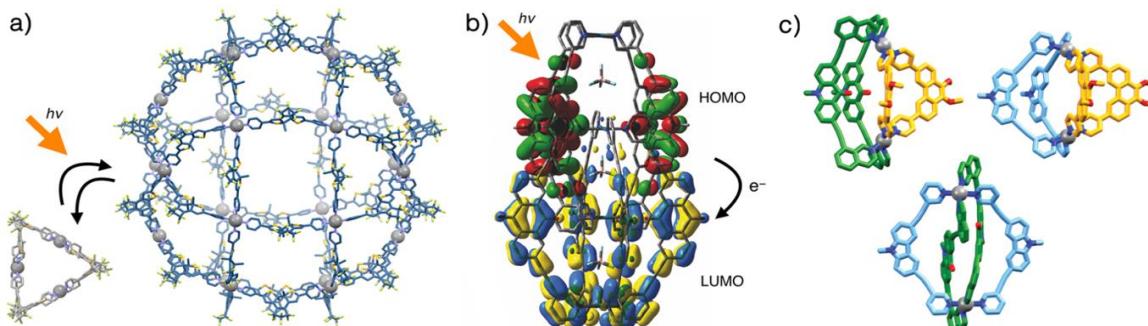
# Non-statistical Assembly of Functional Coordination Cages

Guido H. Clever<sup>1</sup>

guido.clever@tu-dortmund.de

<sup>1</sup> Fakultät für Chemie und Chemische Biologie, Technische Universität Dortmund, Germany

Advanced self-assembly strategies enable the targeted synthesis of supramolecular systems and materials with increasing structural and functional complexity. We use bis-monodentate ligands, reacting with transition metal cations such as Pd(II) to coordination compounds with a broad range of topologies from small  $Pd_2L_4$  cages, their interpenetrated dimers, rings of various size up to large  $Pd_{24}L_{48}$  spheres.<sup>1</sup> We introduce stimuli-responsive behaviour triggered by small molecules or light leading to the modulation of guest affinity<sup>2</sup> or complete structural reorganization (Figure a).<sup>3</sup> Interpenetrated double cages consisting of donor and acceptor moieties were shown to undergo light-induced charge separation but suffer from a lack of control over stoichiometry and stereochemistry (Figure b).<sup>4</sup> Therefore, we develop various approaches to control the non-statistical assembly of heteroleptic cages with defined structure and composition (e.g. “geometric shape complementarity”; Figure c).<sup>5</sup> Recently, we established guest-to-host<sup>6</sup> and ligand-to-ligand chirality transfer, monitored by CD and CPL spectroscopy. We further present early results on intra-cage charge and energy transfer.



**Figure:** a), b) Light-responsive and c) heteroleptic coordination cages.

## References

- [1] S. Pullen, G. H. Clever, *Acc. Chem. Res.* **2018**, 51, 3052.
- [2] a) S. Löffler, J. Lübben, L. Krause, D. Stalke, B. Dittrich, G. H. Clever, *J. Am. Chem. Soc.* **2015**, 137, 1060; b) M. Han, R. Michel, B. He, Y.-S. Chen, D. Stalke, M. John, G. H. Clever, *Angew. Chem. Int. Ed.* **2013**, 52, 1319.
- [3] a) R. Zhu, J. Lübben, B. Dittrich, G. H. Clever, *Angew. Chem. Int. Ed.* **2015**, 54, 2796; b) M. Han, Y. Luo, B. Damaschke, L. Gómez, X. Ribas, A. Jose, P. Peretzki, M. Seibt, G. H. Clever, *Angew. Chem. Int. Ed.* **2016**, 55, 445.
- [4] M. Frank, J. Ahrens, I. Bejenke, M. Krick, D. Schwarzer, G. H. Clever, *J. Am. Chem. Soc.* **2016**, 138, 8279.
- [5] a) W. M. Bloch, Y. Abe, J. J. Holstein, C. M. Wandtke, B. Dittrich, G. H. Clever, *J. Am. Chem. Soc.* **2016**, 138, 13750; b) K. Wu, B. Zhang, C. Drechsler, J. J. Holstein, G. H. Clever, *Angew. Chem. Int. Ed.* **2021**, 60, 6403; c) S. Saha, B. Holzapfel, Y.-T. Chen, K. Terlinden, P. Lill, C. Gatsogiannis, H. Rehage, G. H. Clever, *J. Am. Chem. Soc.* **2018**, 140, 17384.
- [6] I. Regeni, B. Chen, M. Frank, A. Baksi, J. J. Holstein, G. H. Clever, *Angew. Chem. Int. Ed.* **2021**, 60, 5673.