## POROUS MATERIALS MADE BY DESIGN: THE DYNAMIC COVALENT CHEMISTRY OF ORGANIC CAGES AND FRAMEWORKS

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Porous nanostructures that arrange chemical function in confined space are promising materials for applications in the fields of heterogeneous (photo)catalysis, molecular recognition, sensing, gas storage or separation, membranes, and organic electronics. Metal-Organic or Covalent Organic Frameworks (MOFs and COFs) and molecular cage compounds are examples of current interest for suchlike functional nanostructures.<sup>[1]</sup> Efficient synthesis of these complex scaffolds can be achieved by subcomponent self-assembly of small organic buildings blocks under dynamic reaction conditions (see Figure 1). Hereby, structure, topology and function are directly encoded in the symmetry and topicity of the precursors and the respective coupling reactions, thus allowing for a *Molecular Design Approach* for tailor-made modifications of materials properties.

In the first part of this talk, I will introduce the basic principles of dynamic covalent chemistry. For a series of covalent organic cages<sup>[2]</sup> and macrocycles derived from functionalized tribenzotriquinacenes,<sup>[3]</sup> size and shape can be controlled by varying the bite angles of the molecular precursors. Furthermore, self-sorting experiments<sup>[4]</sup> for multi-cpmponent mixtures give valuable insight into cage-forming pathways, key intermediates and relative stabilities of the assemblies.

In the second part of the talk, I will discuss several strategies for a spatially precise functionalization of the cages for applications in highly porous materials, supramolecular shadow masks for fullerene functionalization<sup>[5]</sup> and molecular recognition.





## **References:**

- [1] F. Beuerle, B. Gole, Angew. Chem. Int. Ed. 2018, 57, 4850–4878.
- a) S. Klotzbach, S. Scherpf, F. Beuerle, *Chem. Comm.* 2014, 50, 12454–12457; b) S. Klotzbach, F. Beuerle, *Angew. Chem. Int. Ed.* 2015, 54, 10356–10360.
- [3] A. Dhara, F. Beuerle, Synthesis 2018, 50, 2867–2877.
- [4] F. Beuerle, S. Klotzbach, A. Dhara, Synlett 2016, 27, 1133–1138.
- [5] V. Leonhardt, S. Fimmel, A.-M. Krause, F. Beuerle, Chem. Sci. 2020, 11, 8409–8415.