RUHR-UNIVERSITÄT BOCHUM
Fakultät für Chemie und Biochemie

Interdisciplinary Lecture Series
Gemeinsames Kolloquium – Wintersemester 2018/19
In Cooperation with the GRK Confinement-Controlled Chemistry

Thursday, 10.01.2019
17:15 hrs, Lecture Hall HNC 30

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Design and Synthesis of Complex Molecular Architectures through Subcomponent Self-Assembly

Abstract:
Porous materials possessing spatially well-arranged functionalities are promising candidates for applications in the fields of heterogeneous catalysis, sensing, gas storage or separation, and membranes. Metal-Organic or Covalent Organic Frameworks (MOFs and COFs) as well as molecular cage compounds are examples of current interest for suchlike functional materials.[1] Efficient synthesis of these complex molecular architectures is achieved by cross-linking of small organic buildings blocks under dynamic conditions (see Figure 1). Thereby, structure and topology of the assemblies are directly encoded in the symmetry and structure of the building blocks and the respective coupling reactions, thus allowing for a *Molecular Design Approach* to facilitate tailor-made modifications of materials properties. In this talk, I will report on the implementation of functionalized diketopyrrolopyrrole (DPP) derivatives into π–conjugated COFs and the spontaneous self-organization of these crystalline polymers into microtubular assemblies with tube diameters of around 300 nm.[2] Furthermore, I will discuss the size- and shape-selective synthesis of covalent organic cage compounds[3] based on the orthogonal tribenzotriquinacene (TBTQ)[4] scaffold. For reaction mixtures containing two difunctional precursors with different bite angles, various types of self-sorting[5] are observed ranging from the *narcissistic* formation of binary cage mixtures to the *social* assembly of unprecedented multi-component cages. Self-sorting under competitive conditions and specific cage-to-cage transformations give insights into both kinetic and thermodynamic stabilities of these dynamic covalent assemblies. For the smallest [2+3]-cage, strong 1:1 complexes with C_{60} or C_{70} are formed and the exohedral fullerene reactivity can be modulated via encapsulation.

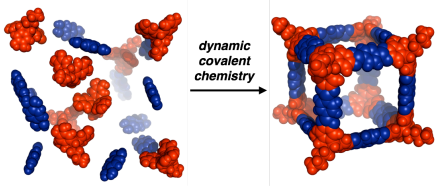

Figure 1: Dynamic covalent self-assembly of small organic building blocks into complex molecular architectures.

Gäste sind herzlich willkommen – Guests are most welcome!

gez. Ch. Hättig	gez. K. Morgenstern	gez. St. Huber
GSCB	Dekanin	GDCH

References:

[1] a) A. G. Slater, A. I. Cooper, *Science* **2015**, *348*, 988; b) F. Beuerle, B. Gole, *Angew. Chem. Int. Ed.* **2018**, *57*, 4850–4878.

[2] B. Gole, V. Stepanenko, S. Rager, M. Grüne, D. D. Medina, T. Bein, F. Würthner, F. Beuerle, *Angew. Chem. Int. Ed.* **2018**, *57*, 846–850.

[3] 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.

[4] A. Dhara, F. Beuerle, *Synthesis* **2018**, *50*, 2867–2877.

[5] F. Beuerle, S. Klotzbach, A. Dhara, *Synlett* **2016**, *27*, 1133–1138.