RTG 2861 "Planar Carbon Lattices" Joint On-site Meeting in Erlangen, November 14-15, 2024

FAU Erlangen-Nürnberg, Südgelände, Seminar room 13301.00.111 (Chemikum Organische Chemie), Nikolaus-Fiebiger-Str. 10 (Access: Erwin-Rommel-Straße 35, Ground floor)

https://maps.app.goo.gl/xyfBxThiXmvCEBpd6

Meeting program

Thursday, 14.11.2024, Seminar room 13301.00.111 (Chemikum Organische Chemie)

12:30 - 13:30 *Joint lunch and welcome coffee*

13:30 - 13:35 Opening remarks

13:35 - 14:05 Progress report: **Shreya Garg**, Project B3, FAU

14:05- 15:00 Subgroup meetings of DR + PI supervisor + PI co-supervisor + collaboration partner;

- Feedback on annual written reports;
- Planning of lab-rotations/ research visits
- Individual discussions with the guest speaker

15:00 - 15:30 Progress report: **Aleena Jose**, Project A4, TUD

15:30 - 16:00 *Coffee break*

16:00 - 17:00 Guest talk by **Prof. Thomas Bein** (LMU),
Talk title: **"Photons, excitons and electrons in covalent organic frameworks"**

Time TBA Joint dinner at Restaurant Grauer Wolf (Hauptstraße 80-82, 91054 Erlangen, https://maps.app.goo.gl/TBvLNr2z8TysfFkd8)

Friday, 15.11.2024, Seminar room 13301.00.111 (Chemikum Organische Chemie)

09:30 - 11:00 Open Book Session

11:00 - 11:30 *Coffee break*

11:30 - 12:30 Remaining discussions & Closing remarks

12:30 - 13:30 *Joint lunch and departure*

RTG-PCL guest talk | Nov 14, 2024 | 16:00 | Seminar room 13301.00.111 (Chemikum Organische Chemie, FAU) and online

Photons, excitons and electrons in covalent organic frameworks

Thomas Bein

Department of Chemistry and Center for NanoScience, University of Munich (LMU), Butenandtstr. 5-13, 81377 Munich, Germany

Covalent organic frameworks (COFs) can be formed through the condensation of molecular building blocks into 2D and 3D crystalline structures. These can include photoactive elements like porphyrins, enabling the creation of well-defined organic bulk heterojunctions, chemical sensors, photocatalysts and photoelectrochemical electrodes (1). Key strategies aim to develop electroactive networks for light-induced and electrochemical charge transfer. For instance, earlier COF-based heterojunctions demonstrated thienothiophenebased donor networks with 3 nm pores, showing charge transfer to an intercalated fullerene acceptor. New donor-acceptor COF phases, using dibenzochrysene-based units with tight π-stacking, show improved interpenetration and charge transfer.

Alternative COF designs stack donor and acceptor molecules in alternating columns forming integrated heterojunctions, promoting charge carrier generation. Other synthetic efforts have produced COFs with extended chromophores for harvesting visible and near-infrared light, and enabling fine-tuned absorption and luminescence. Thin film growth methods have been developed for solvent-stable 2D COF structures, which have potential in photoelectrochemical water splitting. COFs with Wurster-type motifs exhibit high electronic conductivity, while COF films also show great promise as solvatochromic sensors, photodetectors, and feature fast electrochromic response.

Unlike metal-organic frameworks (MOFs), few guest-responsive COF structures exist. Recently, we have developed dynamic 2D COFs that expand or contract based on guest presence, while maintaining high crystalline order (2). These “wine rack” COFs, with π-stacked columns of perylene diimides and flexible bridges, exhibit stepwise transformations with significant volume changes, allowing modulation of excitonic coupling. Ongoing efforts focus on ultra-large pore donor-acceptor COFs with expanded light-harvesting and charge separation capacities, broadening their optoelectronic functionality.

(1) Blätte, Ortmann, Bein, *J. Am. Chem. Soc*. 2024, in press.

(2) Auras et al., *Nat. Chem.* 2024*, 16, 1373.*

Thomas Bein Biographical Sketch

Thomas Bein received his PhD in Chemistry from the University of Hamburg (Germany) and the Catholic University Leuven (Belgium) in 1984. He continued his studies as Visiting Scientist at the DuPont Central Research and Development Department in Wilmington, DE (USA). From 1986 to 1991 he was Assistant Professor of Chemistry at the University of New Mexico in Albuquerque (USA). In 1991 he joined Purdue University (Indiana) as Associate Professor, and was promoted to Full Professor of Chemistry in 1995. In 1999 he was appointed Chair of Physical Chemistry at the University of Munich (LMU), where he also served as Director of the Department of Chemistry.

His work has been recognized by several awards, including an ERC Advanced Grant focusing on Covalent Organic Frameworks. He has been co-founder and LMU-Coordinator of two national Excellence Clusters, including "*e*-conversion". Bibliographic data: > 500 publications, > 60.000 citations, h=127. Since 2018, Thomas Bein has been listed as a Highly Cited Researcher (Clarivate).

His current research interests cover the synthesis and physical properties of functional nanostructures, with an emphasis on molecular frameworks and nanostructured materials for energy conversion applications.

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