RTG 2861 "Planar Carbon Lattices" Joint On-site Meeting in Erlangen, May 16-17, 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, 16.05.2024, 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 - 13:45 Flash presentation: **Johanna Krüger** (associated DR | Hirsch group @FAU)

13:45 - 13:55 Flash presentation: **Tamara Nagel** (associated DR | Hirsch group @FAU)

14:00- 16:00 Lab tours at FAU (jointly with SolTech network, visits to Spieker/Brabec/Bachmann groups) - **DRs only**

16:00 - 16:30 *Coffee break*

16:30 - 17:30 Guest talk by **Prof. Jong-Beom Baek** (UNIST, Korea),
Talk title: "Mechanochemistry for sustainable materials synthesis"

19:15 Joint dinner at Kitzmann BräuSchänke (Südliche Stadtmauerstraße 25, 91054 Erlangen)

Friday, 17.05.2024

09:30 - 11:00 Elektronikpraktikum, Physikum Staudtstr. 7, entrance B3, room 00.572/00.573
Session on Electronic Lab Notebooks by **Prof. Heiko Weber** and **Dr. Michael Krieger** (30 min presentation + 60 min hands-on training in teams of two)

Seminar room 13301.00.111 (Chemikum Organische Chemie)

11:00 - 11:30 *Coffee break*

11:30 - 12:00 Progress report: **Paul-Alexander Laval-Schmidt**, Project A1, TUD

12:00 - 12:30 Remaining discussions & Closing remarks

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

RTG-PCL guest talk | May 16, 2024 | 16:30 | Seminar room 13301.00.111 (Chemikum Organische Chemie, FAU) and online

Mechanochemistry for sustainable materials synthesis

Prof. Dr. Jong-Beom Baek

Center for Dimension-Controllable Organic Frameworks (CDCOF), 50 UNIST, Ulsan 44919, Korea

Conventional reactions are mostly driven by heat, light, and electricity. They are named as thermochemistry, photochemistry, and electrochemistry, respectively. Likewise, chemical reaction, caused by mechanical actions, is defined as mechanochemistry, which delivers energies required to overcome reaction barriers via abrasion, friction, cracking, colliding, and so on. The most representative tool for operating mechanochemistry is ball-milling, which can offer a new avenue for sustainable materials synthesis, including (1) single atom catalysts (SACs) from bulk metal balls, (2) methane from char coals, and (3) ammonia from nitrogen. Various SACs can be produced by a top-down mechanochemical abrasion method, in which the bulk metal balls (single atom percussors) are directly atomized onto different substrates, such as carbon frameworks, oxides, carbides, and nitrides.[1] Carbon frameworks, such as char coals in the presence of hydrogen (carbon hydrogasification), can also be efficiently converted into methane via mechanochemical ball-milling.[2] The rate of carbon hydrogasification is four orders of magnitude higher than the conventional thermochemical method. Furthermore, ammonia has mainly been produced by the Haber-Bosch process over 110 years. However, it cannot be performed under mild conditions, because of thermodynamic reasons. We have discovered a new method for the synthesis of the ammonia under mild conditions (45 °C and 1 bar) via mechanochemical ball-milling iron (Fe) catalyst in the presence of nitrogen and hydrogen.[3] With this new process with potassium (K) promoter, the final concentration of ammonia have reached as high as 94.5 vol%,[4] which is nearly 4 times higher than the state-of-art Haber-Bosch process (~25 vol%) under harsh conditions (450 °C and 200 bar). Stable nitrogen dissociation at the mild conditions is associated with mechanochemically induced high defect density and violent mechanical actions on the Fe catalyst.[5]

1. Han, et al., Nature Nanotechnology 17 (2022), 403-407.
2. Han, et al., Angew. Chem. Int. Ed. 61 (2022), e202117851.
3. Han, et al., Nature Nanotechnology 16 (2021), 325-330.
4. Kim & Han, et al., Nature Communications 14 (2023), 2319.
5. Han, et al., Science Advances 5 (2019), eaax8275.