

Schedule Retreat Hotel Döllnsee Schorfheide on June 12/13.2025 - Status June 12, 2025 -

| Time | Name | Supervisor(s) | Tentative presentation titles | Batch |
|-------------------------------|---------------------------|--|--|-------------------|
| Thursday 12.6.2025 | | | | |
| 08:30 | Departure per bus | | Meeting point: 08:10 between old chemistry building and main building of TU | |
| 10:30 | Arrival Hotel – Room | | Moderation: Maria-Andrea | |
| 10:50-11:20 | Elizaveta | Horch/Weber | Understanding catalyst reactions by time-resolved spectroscopy and mathematic modelling | WS22 |
| 11:20-11:50 | Denise | Mroginski/Horch | Does it take two CO? Probing acetyl-CoA synthase under ambient conditions with ultrafast IR and anharmonic calculations | WS23 |
| 11:50-12:20 | Laura | Nürnberg/Zou ni/Scheerer | Improved photosystem coupling and a novel spectral-tuning approach in light driven formate production | WS23 |
| 12.20-13:30 | Lunch | | Moderation: Oli | |
| 13:30-14:00 | Maria | Heberle/Mroginski | Infrared spectroelectrochemistry studies on a bifurcating electron transferring flavoprotein | WS22 |
| 14:00-14:30 | Anushka | Dobbek/Zebger | Design of artificial metalloenzyme for CO2 reduction and CC-coupling reactions | WS22 |
| 14:30-15:00 | Zishuo | Zebger/Mroginski | Elucidating structure and electronic properties of the double cubane cluster protein by vibrational spectroscopy and quantum chemical computations | WS23 |
| 15:00-15:20 | Coffee break | | Moderation: Juri? | |
| 15:20-15:50 | Enlin | Sun/Roderer/Lange | Structural investigation of rhomboid proteases by cryo-EM” | WS23 |
| 15:50-16:20 | Francisco | Neubauer/Lenz | Development and scale-up of a fed-batch process for heterologous hydrogenase production in <i>E. coli</i> | WS22 |
| 16:20-16:50 | Jonas | Neubauer/Sun | Identification and characterization of halogenases acting on nucleoside scaffolds | WS23 |
| 16:50-17:00 | Short online presentation | Carsten Krebs, Martin Bollinger, and Amie Boal | https://sites.psu.edu/bollingerkrebsgroup/ https://sites.psu.edu/boalgroupp/ | Penn. State Univ. |
| 17:00-17:20 | Coffee break | | Moderation: Adam & Ana | |
| 17:20-18:50 | Workshop | Adam Belsom, Ana Perez | PhD acceleration: „Writing” – Part 1 | |
| and parallelly> | | | | |
| 17:20 -19:00 | Discussion among Pls | All present Pls | Ideas for future collaboration – among others “PhD2Startup” concept | |
| 19:00-20:00 | Dinner | | | |
| 20:00-22:30 | Interactions | | | |

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| Friday 13.6.2025 | | | Moderation: Martin (Oestreich) | |
| 09:00-09:30 | Yao | Oestreich | Enantioselective desymmetrization of 1,1'-biaryl-2,6-dinonaflates by palladium-catalyzed C(sp ²)-B cross-coupling with B-B reagents | WS22 |
| 09:30-10:00 | Xiaojie | Oestreich | One-pot sequential alcohol activation and nickel-catalyzed cross electrophile coupling with chlorosilanes | WS23 |
| 10:00-10:30 | Yaxin | Gurlo/ Schomäcker/ Hess | Polymer assisted synthesis of intermetallic catalysts for energy conversion and storage | WS22 |
| 10:30-10:50 | Coffee break | | Moderation: Reinhard | |
| 10:50- 11:20 | Warisha | Thomas/Bojdys | Rational Design of Core-Shell Catalysts for Selective Nitrate-to-Ammonia Conversion | WS22 |
| 11:20-11:50 | Camila | Al Naji/Neubauer/ Antonietti | Biomass fractionation for the upgrading of sugars and its derivatives to platform chemicals | WS23 |
| 11:50 – 13:00 | Lunch | | Moderation: Reinhard | |
| 13:00-13:30 | Badr | Hess | An atomistic model for surface corrosion of RuO ₂ -based electrocatalysts for the acidic oxygen evolution reaction | WS22 |
| 13:30-14:00 | Daniil | Nunes Alves/Leimkühler/ Antonietti | Using deep learning and machine learning-based docking to investigate enzyme-substrate complexes | WS23 |
| 14:00-14:20 | Coffee break | | Moderation: Adam & Ana | |
| 14:20-16:20 | Workshop | Adam Belsom, Ana Perez | PhD acceleration: „Writing” – Part 2 | |
| 16:30 | Departure by bus | | | |
| Approx. 17:30/18:00 | Berlin | | | |