



Annual Workshop

27-29 September 2023

Hotel Kloster Nimbschen – Nimbschener Landstraße 1 – 04668 Grimma

Wednesday, 27 September

doctoral researchers (DRs) only

09:30 – 10:00 Welcome and organisational matters

10:00 – 10:30 *Coffee break*

10:30 – 12:30 Physical activity

12:30 – 13:30 *Lunch*

13:30 – 15:15 **Invited talk (with many questions)**
Chad Elmore (Head of Isotope Chemistry, AstraZeneca)
title

15:15 – 16:00 *Coffee break*

16:00 – 18:30 Poster session with assignments

18:30 – 19:30 *Dinner*

20:00 – 22:00 Bowling

Thursday, 28 September

all RTG members

06:30 – 09:00 *Breakfast*

09:00 – 09:10 Welcome remarks by the spokesperson

09:10 – 09:45 **Invited talk (25+10)**
Chad Elmore (Head of Isotope Chemistry, AstraZeneca)
title

09:45 – 10:45 **Progress report (12+8 each) session 1 (chair: Patricia Seidel)**
Jonathan Lebelt (P10)
Selective electrochem. reduction of ketones using a cathode-shielding electrolyte
Marie van der Loh (P11a)
Analysis of a particle catalyzed reaction in a single droplet using ESI/MS
Jannik Sälker (P9)
Photocatalytic activation and deuteration of small organic molecules

10:45 – 11:15 *Coffee break*

11:15 – 12:15 **Progress report session 2 (chair: Milena Barp)**

Sophia Leippe (P1a)

Characterization of a nanoparticle mass spectrometer

Shabnam Haque (P1)

IRPD study of cationic copper complexes investigating H₂/D₂ binding

Elvira Gouatieu Dongmo (P2)

Computational modelling of atomistic motifs for adsorptive H₂ isotopologue separation

12:15 – 13:30 *Lunch*

13:30 – 14:30 **Progress report session 3 (chair: Robert Schiewe)**

Raza Ullah Khan (P14)

Quantifying hydrogen isotope effects on chemical bonding

Florian Kreuter (P14a)

Energy decomposition analysis (EDA) for excited states

Robert Temme (P7)

Catalyst-assisted hydrogen isotope separation through membranes

14:30 – 16:00 *Coffee break and free time*

16:00 – 17:00 **Progress report session 4 (chair: Konstantin Marcinowski)**

Alexandra Becker (P12)

Towards miniaturization of LSC using microfluidic methods combined with potential modification of graphene defect structures owing to electron irradiation

Sibo Chetry (P3)

Designing defect-engineered Cu-paddle-wheel MOFs for H isotope separation

Muhammad Fernadi Lukman (P5)

Monitoring the isotope-selective response of flexible metal-organic frameworks toward the adsorption of dihydrogen isotopes

17:00 – 19:00 **Poster session**

19:00 – 20:00 *Dinner*

20:00 – 23:00 **Informal discussions**

Friday, 29 September

DRs, PIs

06:30 – 09:00 *Breakfast*

09:00 – 10:15 **Annual Report and discussion**

10:15 – 10:45 *Group photo and coffee break*

10:45 – 12:00 **PI meeting (PIs) / Doctoral Forum (DRs)**

12:00 – 12:45 *Lunch and departure*
