

2025 Annual Retreat of the Atomistic Modelling Center

	Tuesday 22.07.2025	Wednesday 23.07.2025	Thursday 24.07.2025
08:00		breakfast Hotel Burgblick	breakfast Hotel Burgblick
08:15			
08:30		by foot 8 min. to Stadtplatz Burghausen	by foot 8 min. to Stadtplatz Burghausen
08:45		Shuttle-Bus to Raitenhaslach, 10 min.	08:58, 09:28 to go ca. 8 min to train station
09:00	09:07 departure München Hbf Gleis 8	Casper Larsen	Bahnhof Burghausen
09:15			(by Citybus 1 Blue Line, every 30 min.)
09:30		Prajwal Pisal	
09:45			09:45 departure Burghausen Bahnhof Gleis 1
10:00		Martin Schwade	
10:15	10:17 arrival Mühldorf Gleis 3 A-B		10:21 arrival Mühldorf Gleis 2 C-G
10:30	10:37 departure Mühldorf Gleis 2 A-B	Coffee break	10:30 departure Mühldorf Gleis 3 C-F
10:45			
11:00		Waldemar Kaiser	
11:15	11:16 arrival Burghausen Gleis 1		
11:30	Shuttle-Bus Burghausen Bahnhof directly to	Michal Sanocki	11:37 arrival München Hauptbahnhof Gleis 6
11:45	Raitenhaslach (incl. luggage), 10 min.		
12:00		Weilong Chen	
12:15	Welcome		
12:30	Lunch at Akademiezentrum Raitenhaslach	Lunch at Akademiezentrum Raitenhaslach	
12:45			
13:00			
13:15			
13:30			
13:45	Manuel Grumet	Workshop w. Heidi Henrickson Pls parallel:	
14:00		Annual General	
14:15	Alessandro Mangiameli	Meeting	
14:30			
14:45	Mohammad Rahbar		
15:00			
15:15			
15:30	Coffee break	Coffee break	
15:45			
16:00	Poonam	Workshop w. Heidi Henrickson Pls parallel:	
16:15		Strategy Meeting	
16:30	Zhaosu Gu		
16:45			
17:00	Maximilian Dorfner		
17:15			
17:30	Konrad Merkel		
17:45		Shuttle-Bus to Burghausen Stadtplatz 10 min.	
18:00	Dinner at Klosterhof Raitenhaslach	Dinner at Hotel Post Burghausen	
18:15			
18:30			
18:45			
19:00			
19:15			
19:30			
19:45			
20:00			
20:15	Shuttle-Bus to Burghausen Stadtplatz 10 min.	by foot ca. 8 minutes	
20:30	by foot ca. 8 minutes	Hotel Burgblick, Ach	
20:45	Hotel Burgblick, Ach		

Tuesday 22.07.2025

12:15-12:30 Welcome

12:30-13:45 *Lunch at Akademiezentrum Raitenhaslach*

13:45-14:15 *Equivariant Neural Network Machine Learning for Dynamic Electronic Structure*
Manuel Grumet (Prof. Egger)

14:15-14:45 *Rigorous Benchmark of Implicit Electrolyte Models*
Alessandro Mangiameli (Prof. Stein)

14:45-15:15 *A strongly coupled system perspective on hybrid solvation models*
Mohammad Rahbar (Prof. Stein)

15:30-16:00 *Coffee break*

16:00-16:30 *Computational Screening of Potential Metal Nanocluster Precursors for ZIF-8 Encapsulation*
Poonam (Prof. Gagliardi)

16:30-17:00 *Accelerating Molecular Energy Prediction via DimeNet-Transformer-GP Fusion*
Zhaosu Gu (Prof. Gagliardi)

17:00-17:30 *Modeling Electron-Vibrational Interactions: From Ab Initio Parameterization to Tensor Network Methods*
Maximilian Dorfner (Prof. Ortmann)

17:30-18:00 *Optical properties for large systems using the linear scaling Wannier optics approach*
Konrad Merkel (Prof. Ortmann)

18:00-20:15 *Dinner at Klosterhof Raitenhaslach*

Wednesday 23.07.2025

08:00-08:30	<i>breakfast Hotel Burgblick</i>	
09:00-09:30	<i>Machine Learning Potentials for Prior Estimation and Multifidelity Sampling in Global Atomic Structure Optimization</i> Casper Larsen (Prof. Rinke)	
09:30-10:00	<i>Machine Learning Accelerated Descriptor Design for Catalyst Discovery in CO₂ to Methanol Conversion</i> Prajwal Pisal (Prof. Rinke)	
10:00-10:30	<i>Physics-informed kernel-based machine learning for finite-temperature Hamiltonians</i> Martin Schwade (Prof. Egger)	
10:30-11:00	<i>Coffee break</i>	
11:00-11:30	<i>Identifying Mobile Ions in Solid Electrolytes from Machine Learning Potentials and Raman Spectroscopy</i> Waldemar Kaiser (Prof. Egger)	
11:30-12:00	<i>Learning Non-Local Molecular Interactions via Equivariant Local Representations and Charge Equilibration</i> Michal Sanocki (Prof. Zavadlav Koller)	
12:00-12:30	<i>From Training to Deployment: Scalable Molecular Dynamics with Machine Learning Potentials</i> Weilong Chen (Prof. Zavadlav Koller)	
12:30-13:45	<i>Lunch at Akademiezentrum Raitenhaslach</i>	
13:45-15:30	<i>Poster presentation workshop</i> Workshop with Heidi Henrickson	<i>Annual General Meeting</i> PIs parallel
15:30-16:00	<i>Coffee break</i>	
16:00-17:45	<i>Pitching your next manuscript to your research group leader</i> Workshop with Heidi Henrickson	<i>Strategy Meeting</i> PIs parallel
18:00-20:15	<i>Dinner at Hotel Post Burghausen</i>	

Thursday 24.07.2025

08:00-08:30 ***breakfast Hotel Burgblick***