

RTG 2861 “Planar Carbon Lattices” Joint On-site Meeting in Erlangen, May 11-13, 2026

Location: FAU, Südgelände, Seminar room 13301.00.111 (Chemikum Organische Chemie), Nikolaus-Fiebiger-Str. 10 (Access: Erwin-Rommel-Straße 35, Ground floor), 91058 Erlangen

Meeting program

Time		Mon (May 11)	Tue (May 12)	Wed (May 11)			
		for all	for all	For DRs	For Pls & Coord		
09:00	09:00		Timeline Submission Proposal + Progress Report 2FP	Lab tours for DRs	If needed: Additional discussions/Planning (Time can be adjusted)		
	09:15		A1, Feng: Project proposal 2FP (online)				
09:30	09:30		A2, Niu: Project proposal 2FP				
	09:45		A3, Hauke: Project proposal 2FP				
10:00	10:00		A4, Kaskel: Project proposal 2FP (online)				
	10:15		B1: Halik, Project proposal 2FP				
10:30	10:30		B2: Heine, Project proposal 2FP				
	10:45		C4: Maultzsch, Project proposal 2FP				
11:00	11:00		<i>Coffee break</i>				
	11:15						
11:30	11:30		C3: Guldi, Project proposal 2FP				
	11:45		C5: Weidinger, Project proposal 2FP (online)				
12:00	12:00	B4: Weber, Project proposal 2FP	Closing discussion & remarks - 15min				
	12:15	Arrival	Time for wrap-up remarks				
12:30	12:30	<i>Lunch</i>	<i>Lunch</i>	<i>Lunch</i>			
	12:45						
13:00							
13:00	13:00	Departure					
	13:15						
13:30	13:30	Progress report 1: Britta Maib (C4, Maultzsch)	Guest talk 2 (Dr. A. Cangi, HZDR/CASUS)				
	13:45						
14:00	14:00	Progress report 2: Jiwon Byun (B1, Halik)					
	14:15						
14:30	14:30	Progress report 3: Anu Joseph (C5, Weidinger)	Progress report 4: Kevin Gerein (A3, Hirsch)				
	14:45						
15:00	15:00	<i>Coffee break</i>	<i>Coffee break</i>				
	15:15						
15:30	15:30	Guest talk 1 (Prof. C. Müller, FAU)	Discussion Progress Report				
	15:45						
16:00	16:00	Hobby project & Other Discussions	Hobby project & Other Discussions				
	16:15						
16:30	16:30						
	16:45						
17:00	17:00						
	17:15						
17:30	17:30						
	17:45						
18:00	18:00						
	18:15						
18:30	18:30	<i>Group dinner (JINH)</i>					

Lab tours on Wednesday (May 13)

Start Time Labtours	Group 1	Pausen/Laufzeit	Group 2
09:00	Spieker	30 min	Steinrück
09:30		5-10 min	
09:35	Guldi	30 min	Spieker
10:05		10 min	
10:15	Steinrück	30 min	Guldi
10:45		10-15 min	
11:00	Maier	30 min	Maultzsch
11:30		5 min	
11:35	Maultzsch	30 min	Maier
12:00	Back to the seminar room		

From Twisting Motions to Function: Towards Design Principles for Photoactive Molecules

C. Müller, Erlangen/GER

Jun.-Prof. Carolin Müller, Friedrich-Alexander-Universität Erlangen-Nürnberg,
Computer-Chemistry-Center, Nögelsbachstraße 25, 91052 Erlangen

Understanding how photoexcitation reshapes a molecule's geometric and electronic structure is key for the rational design of responsive functional molecules and materials. In this talk, I will present theoretical studies on molecular systems that undergo pronounced conformational changes in the excited state, such as molecular switches and twisted intramolecular charge transfer (TICT) systems. The emphasis will be on the interplay between quantum chemical simulations and (time-resolved) spectroscopy, particularly (transient) IR and UV/Vis absorption techniques, examining how these methods jointly reveal how structural twisting influences transient spectroscopic features, and how this understanding can be translated into practical design principles.

Short Curriculum Vitae

I am a chemist passionate about unraveling the mysteries behind the behavior of photoexcited molecules using quantum chemical-, cheminformatical- and spectroscopic methods.



since 11/2023	Juniorprofessor for the Theory of Electronically Excited States, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany
06/2022–10/2023	Feodor Lynen Postdoctoral Researcher, University of Luxembourg, Luxembourg
03/2021–05/2022	Postdoctoral Researcher, Friedrich Schiller University Jena, Germany
09/2018–02/2021	Dissertation (Dr. rer. nat), Friedrich Schiller University Jena, Germany
10/2013–09/2018	B. Sc. and M. Sc. in Chemistry, Friedrich Schiller University Jena, Germany

When Do Machine Learning Models Learn Chemistry? From Electronic Structure to Latent Space Steering

Dr. Attila Cangi, Center for Advanced Systems Understanding (CASUS), Helmholtz-Zentrum Dresden-Rossendorf (HZDR)

Recent advances in machine learning are reshaping how we model and understand matter across scales—from electronic structure in materials to the chemical property spaces of molecules. In this talk, I present two complementary approaches that illustrate how data-driven models can both accelerate simulation and enable control over complex chemical systems.

First, I introduce the Materials Learning Algorithms (MALA) framework, a scalable machine learning approach for predicting electronic structure in large-scale atomistic simulations. By leveraging local descriptors of atomic environments, MALA efficiently approximates key electronic observables, including the local density of states, charge density, density of states, and total energy, enabling density functional theory-level insights at significantly reduced computational cost. Applications to diverse systems including boron clusters, liquid-solid aluminum interfaces, and extended defects in beryllium demonstrate its versatility and scalability.

In the second part, I shift focus from atomistic simulation to molecular generative modeling, examining how latent representations learned by transformer-based variational autoencoders can encode chemically meaningful structure. I address a central challenge in this domain: the risk that apparent structure-property relationships are driven by superficial sequence statistics rather than underlying chemistry. To disentangle these effects, I introduce a framework for identifying and validating latent directions associated with distinct molecular properties. By combining linear and nonlinear probing with decoded-molecule validation, we demonstrate robust and controllable steering of properties such as lipophilicity and polarity.

Short Curriculum Vitae

Attila Cangi is Head of the Department of Machine Learning for Materials Design at the Center for Advanced Systems Understanding (CASUS), Helmholtz-Zentrum Dresden-Rossendorf (HZDR). He leads a research team focused on applying artificial intelligence and machine learning to computational materials modeling. Their work centers on developing scalable methods that accelerate first-principles simulations of electronic and atomistic structures as well as advanced models for chemical property prediction, with the overarching goal of discovering and designing novel materials. Attila Cangi earned his Ph.D. in Chemistry from the University of California, Irvine. He previously held positions as a postdoctoral fellow at the Max Planck Institute of Microstructure Physics and as a staff scientist at Sandia National Laboratories.