

Southern Lower Saxony Theoretical Chemistry Meeting
Seminar on Computational Chemistry
Leibniz University Hannover
June, 10th 2026

10:00	Arrival & Coffee	OCI Library
11:00	Welcome	Walsrode Lecture Hall
11:10	Lynn Meeder (Göttingen) The Self Consistent Tangent Nudged-Elastic Band Method for Reaction Pathway Modeling	Walsrode Lecture Hall
11:30	Grace Hsiao-Han Chuang (Hannover) Decoding Chemical Reaction Bifurcations via Newton Trajectories and Autoencoders	Walsrode Lecture Hall
11:50	Wadtey Oung (Braunschweig) Assessing Vibrational Frequency Calculations: From Benchmarking to Blind Predictions	Walsrode Lecture Hall
12:15	Snacks and Posters	OCI Library
14:10	Anna van Bodegraven (Braunschweig) Benchmarking of Vibrational Exciton Models Against Quantum-Chemical Localized-Mode Calculations	Walsrode Lecture Hall
14:30	Katharina Rütter / Carolin König (Hannover) Subsystem Vibrational Coupled Cluster Response Theory	Walsrode Lecture Hall
14:50	Henry Snowden (Göttingen) Non-Equilibrium Electron Dynamics in Plasmonic Materials	Walsrode Lecture Hall
15:10	Coffee/Tea break	
15:30	Liza Surzhikova (Braunschweig) Generative Design of Amines for Sustainable CO ₂ Capture	Walsrode Lecture Hall
15:50	Laura Schiebel (Göttingen) A Database for Protonic Densities and Energies and Perspectives for Multicomponent Calculations	Walsrode Lecture Hall
16:15	Coffee and Posters	OCI Library
17:15	Reinhard Maurer (Göttingen, GdCh) Deus Ex Machina: Augmenting First Principles Theory with Machine Learning Methods	Walsrode Lecture Hall

Locations:

OCI Library: Institute of Organic Chemistry, Schneiderberg 1b, 30167 Hannover, building 2505, room 145

Walsrode Lecture Hall: Institute of Technical Chemistry, Callinstrasse 3-9 30167 Hannover, building 2501, room 219