Annual Meeting 2025

GAMM activity group **Modelling, Analysis and Simulation of Molecular Systems** (MOANSI)

Institute for Advanced Study, Technische Universität München

Programme

Thursday, 20 November, 2025

10:15-11:00 Registration and Coffee

11:00-11:40 **Stefan Vučković** (Uni Fribourg): Reducing errors in Traditional and Machine-Learned Density Functional Calculations

11:45-12:05 **Jonas Beck** (Uni Stuttgart): On the Regularity of the discretized Coupled Cluster Amplitudes

12:10-12:30 **Thiago Corso** (Uni Stuttgart): A rigorous formulation of density functional theory for electrons in one dimension

12:30-14:00 Lunch break

14:00-14:20 **Mi-Song Dupuy** (Sorbonne): A posteriori error estimates for LCAO basis

14:25-14:45 **Ivan Spirandelli** (Uni Potsdam): Geometric and topological potentials guiding protein self-assembly

14:50-15:10 **Lukas Mayrhofer** (TUM): Coarse-grained simulation of protein self-assembly

15:15-15:35 **Jonas Püschel** (Uni Augsburg): Neural Network Acceleration of Iterative Methods for NL-Schrödinger eigenvalue problems

15:35-15:45 General Assembly

15:45-16:15 Coffee break

16:15-16:35 **Markus Penz** (LMU): Homogeneous Sobolev spaces in Maxwell's equation and density-functional theory

16:40-17:00 **Martin Hermann** (Uni Augsburg): Local convergence of Riemannian optimization methods for rotating multicomponent BECs

17:05-17:25 **Liwei Zhang** (RWTH Aachen): Efficient generation of group-equivariant and permutation-invariant polynomials

17:30-17:50 **Vahid Nateghi** (MPI Magdeburg): Projection-based Coarse Graining for Underdamped Langevin Dynamics

17:55-18:15 **Rafael A. L. Reyes** (Uni Stuttgart): A Numerical Study of the Landau Hamiltonian

19:30 Workshop dinner & scientific exchange (open end)

Friday, 21 November, 2025

09:00-09:40 **Guido Falk van Rudorff** (Universität Kassel): Alchemical Perturbations Characterizing Chemical Space: Interpretability, Intrinsic Dimension and Sampling
09:45-10:05 **Nicholas Gao** (CUSP AI): Accurate Ab-initio Neural-network Solutions to Large-Scale Electronic Structure Problems
10:10-10:30 **Maximilian Reihn** (Uni Suttgart): Predicting Fractures in Disordered Material

10:30-11:00 Coffee break

11:00-11:20 **Alfred Kirsch** (TUM): A mathematical analysis of the discretized IPT-DMFT equations
11:25-11:45 **Mathias Oster** (RWTH Aachen): Universal Approximation of the regularized Lieb functional by neural networks
11:50-12:30 **Christopher Stein** (TUM): Fluctuation relation beyond the Jarzynski equality and solvation models from a probabilistic view on the solute-solvent interaction energy

12:30 Lunch and departures

Scientific organisers:

Gero Friesecke and
Muhammad Hassan

Local organisers:

Gero Friesecke,
Muhammad Hassan,
and Amadeus Dorchholz