universität innsbruck

Department of Mathematics

Mathematics Colloquium

Caroline Lasser

TU München

Numerical analysis for watching chemistry happen

The quantum-mechanical model of molecular dynamics and thus of chemical reactions is the time-dependent Schroedinger equation. Such truely out-of-equilibrium dynamics ask for very flexible numerical methods capable of resolving high dimensionality. We present an overview of state of the art methods, discuss their known mathematical underpinning, and give some recent results on the regularization of the time-dependent variational principle, which is joint work with M. Feischl, C. Lubich, and J. Nick.

May 28, 2024
16:00 – 17:00

HS F, Viktor-Franz-Hess Haus, Technikerstraße 25