

## Seminar:



JOHANNES GUTENBERG  
UNIVERSITÄT MAINZ

---

**Room:** Prof. Sinova's Office, 01-327 (Staudinger Weg 7)

**Time:** October 28th, 2016 at 13:00

## Sebastian Müller

JGU Mainz

## **VOTCA-STP Development: Results for Idealized Systems**

Organic spintronics marries the strengths of spintronics with the unbeatable cost-efficiency and tailorability of organic compounds. In our group, we have developed the first software package for multi-scale modeling of spin dynamics in atomistic models of organic materials, VOTCA-STP.

This package is based on a stochastic kinetic Monte Carlo (KMC) model, with parameters calculated from state-of-the-art first-principles theory. Developing the KMC, originally structured for simulations of charge dynamics only, to include also spin dynamics, has presented a range of unique challenges. Solutions to these will be presented and discussed in detail, along with suggestions for remaining problems and an outlook for the future.

All interested are cordially welcome!