

Seminar über Theoretische Chemie

jeweils donnerstags, 15:30 Uhr, im Seminarraum 408, 4. OG, Geb. 30.44

- 31.10.19** **Dr. Kevin Reiter**
Calculation of metal affinities for the active center in alcohol dehydrogenases
- 14.11.19** **Prof. Dr. Peter Schwerdtfeger (Massey U, New Zealand)**
From the Schrödinger equation to the Dirac equation and beyond
- 28.11.19** **Max Kehry**
One- and two-component damped-response theory
- 05.12.19** **Ansgar Pausch**
Towards a fast and accurate description of molecules in finite magnetic fields
- 12.12.19** **Dr. Christof Holzer**
Current advances in Turbomole for ground- and excited states from DFT
- 16.01.20** **Fabian Mack**
Basis sets for NMR coupling tensors
- 30.01.20** **Nils Schieschke**
Applications of CI methods for excited states and embedded systems
- 13.02.20** **Twinkle Yadav**
Spin-orbit CI calculations for magnetic properties

gez. K. Fink, M.E. Harding, S. Höfener, W. Klopper, F. Weigend