Karlsruher Institut für Technologie

Institut für Physikalische Chemie
Abteilung für Theoretische Chemie

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

23.01.20 **Twinkle Yadav**
Spin-orbit CI calculations for magnetic properties

30.01.20 **Nils Schieschke**
Applications of CI methods for excited states and embedded systems

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