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

18.10.18 **Nils Schieschke**
Configuration-interaction frozen-density embedding

08.11.18 **Ansgar Pausch**
Translational-invariant calculation of oriented CD spectra in the framework of damped response theory

15.11.18 **PD Dr. Ulrich Sternberg (COSMOS GbR, Jena)**
Molecular dynamics driven by tensorial properties – a new way to study molecular structures

22.11.18 **Dr. Tilmann Bodenstein**
Strategies for shortening configuration-interaction expansions

29.11.18 **Dr. Heike Fliegl**
Theoretical studies as a tool for understanding the aromatic character of porphyrinoid compounds

~~**06.12.18 Dr. Stephan Kohaut**~~
~~Structures and properties of small hydrogenated platinum clusters~~

10.01.19 **Yannick Franzke**
NMR shielding tensors in relativistic all-electron theory

17.01.19 **Fabian Mack**
Implementation of nuclear spin coupling constants in TURBOMOLE

24.01.19 **Twinkle Yadav**
Magnetic anisotropy in rare-earth compounds

31.01.19 **Christof Holzer**
Low-scaling two-component *GW*/BSE implementation in TURBOMOLE

gez. K. Fink, W. Klopper, F. Weigend