Karlsruher Institut für Technologie

Institut für Physikalische Chemie
Abteilung für Theoretische Chemie

Seminar über Theoretische Chemie

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

25.04.13 **Judith Reichenbach**
Analytische Ultrazentrifugation zur Charakterisierung von einwandigen Kohlenstoffnanoröhren

02.05.13 **Dr. Michael E. Harding**
Systematic construction of complementary auxiliary basis sets from and for atomic natural orbitals

16.05.13 **Dr. David P. Tew (University of Bristol)**
Local pair natural orbitals in explicitly correlated electronic structure theory

23.05.13 **Dr. Matthew Kundrat**
Towards the description of ground-state charge transfer at organic interfaces with subsystem DFT

29.05.13 **Stella Kritikou (Texas A&M University)**
Theoretical investigation of the reactivity of Ir(II) sulfides:
$Ir_2(\mu\text{-}S)_2(PPh_3)_4$ and $Ir_2(\mu\text{-}S)_2(PH_3)_4$

20.06.13 **Tilmann Bodenstein**
Trinuclear early−late transition metal thiolate complexes

27.06.13 **Jiří Chmela (Institute of Chemical Technology Prague)**
Theoretical study of the hydrated electron: Structure and spectroscopy

04.07.13 **Dr. Markus K. Armbruster**
Parallelization of two-component RIDFT with Global Arrays (GA)

11.07.13 **Hai Anh Tran (Vortrag im Vertiefungspraktikum)**
Active Thermochemical Tables (ATcT)

16.07.13[*)] **Professor Ludwik Adamowicz (University of Arizona, Tucson)**
Very accurate atomic and molecular quantum-mechanical calculations with and without assuming the Born-Oppenheimer approximation

19.07.13[**)] **Dr, Peter Deglmann (BASF SE, Ludwigshafen)**
Quantum chemistry beyond gas-phase reactivity: Prediction of thermodynamics and kinetics for condensed-phase reactions

***) Dienstag, 16:00 Uhr, Rehbock-Hörsaal (HS 59, Geb. 10.81, Otto-Ammann-Platz 1) !**

****) Freitag !**