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

16.04.18[*)] **Prof. Dr. Tomasz A. Wesolowski (Universität Genf)**
Frozen-density embedding theory: From the general formulation to practical simulations

19.04.18 **Florian Rehak (HU Berlin)**
Ab initio studies of Brønsted site heterogeneity and its influence on catalytic performance of H-MOR zeolite – Test of different density functionals for molecule–surface interaction

26.04.18 **Kevin Reiter**
Latest developments in the module MPSHIFT and magnetically induced ring currents in toroidal carbon nanotubes

17.05.18 **Christof Holzer**
Implementation of two-component *GW*/BSE theory in TURBOMOLE

24.05.18 **Xin Gui**
Application of *GW*/BSE theory to transition-metal complexes

14.06.18 **Max Kehry**
Ab initio computation of Förster resonance energy transfer

28.06.18 **Prof. Dr. Konrad Patkowski (Auburn University)**
New developments in symmetry-adapted perturbation theory

05.07.18 **Nils Schieschke**
CI Embedding

19.07.18 **Asfaw Yohannes**
DFT calculation of CO and O_2 adsorption on Pt nanoparticles: Size effects

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

[a)] **Montag, 16.04.2018, 15:30 Uhr, Seminarraum 408, 4. OG, Geb. 30.44.**