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

30.10.14 **Christopher Stein (U Göttingen)**
Highly accurate theoretical rovibrational spectroscopy of the linear molecules *l*-C_3H^+ and C_4

13.11.14 **Dr. Marco Marazzi (Theoretische Chemische Biologie, KIT)**
Effects of peptide induced forces on the photochemistry of a retinal-like switch

20.11.14 **Dr. Markus Armbruster**
Intermolecular interactions: The energy decomposition analysis

27.11.14 **Dr. Florian Bischoff (HU Berlin)**
Regularizing singularities in electronic-structure calculations

04.12.14 **Dr. Michael Harding**
Systematic construction of auxiliary basis sets from and for atomic natural orbital basis sets

11.12.14 **Jiří Chmela**
Using alkaline earth metals to modulate the photoluminescence of a europium chelate

07.01.15[*)] **Dr. Daniel Friese (U Tromsø)**
Higher-order non-linear and chiroptical molecular properties

15.01.15 **Dr. Thomas-Christian Jagau (U Southern California, Los Angeles)**
Equation-of-motion coupled-cluster methods for metastable states

05.02.15 **Tilmann Bodenstein**
Efficient calculation of spin-orbit coupled multi-configurational states

12.02.15 **Christof Holzer (Universität Graz)**
Ab initio studies on the spectroscopy of trivalent lanthanide ions: Characteristics and challenges

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

*) Mittwochseminar (13:30 Uhr) im Institut für Nanotechologie (INT), KIT-Campus Nord.