

# Seminar über Theoretische Chemie

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

- 28.04.11**     **Alexander Baldes**  
Acceleration of self-consistent-field convergence by combining conventional diagonalization and a diagonalization-free procedure
- 05.05.11**     **Patrik Pollak**  
Lokalisierte Molekülorbitale
- 12.05.11**     **Konstantinos Vogiatzis**  
Interference-corrected explicitly-correlated second-order perturbation theory
- 19.05.11**     **Andreas Fuchs**  
A polarizable QM/MM approach for the calculation of interface properties of organic solar cells
- 26.05.11**     **Rebekka Gulde**  
QZVP-Basissätze für Lanthanoiden
- 09.06.11**     **Adam Kubas**  
Characterization of unusual bonds in some Ge and Sn metalloid clusters
- 16.06.11<sup>\*)</sup>**     **Professor Debashis Mukherjee** (IACS, Kolkata, Indien)  
State-specific multireference coupled-cluster methods: A survey of some recent developments
- 30.06.11**     **Dr. Angela Bihlmeier**  
Computational structure determination of plakotenin
- 07.07.11**     **Dr. Ericka Barnes**  
Computational investigation of intersystem crossing in rhodamine ions

gez. W. Klopper

**\*) Ausnahmsweise um 10:15 Uhr.**