



Seminar über Theoretische Chemie

jeweils donnerstags, 15:15 Uhr, im Seminarraum 311 (Geb. 30.43)

- 17.11.05** **Dr. John McKelvy (Fort Wayne, Indiana, USA)**
A Semiempirical TD-HF Study of UV-Vis Absorption and Emission Properties
- 24.11.05** **Robert Barthel (TU Dresden)**
Computational Study of Interstellar Hydrocarbon Formation
- 01.12.05** **Prof. Dr. George Froudakis (University of Crete)**
NanoCAD - Computer Aided Nanomaterial Design
- 08.12.05** **Rafal Bachorz**
Stabilization of Very Rare Tautomers of Uracil by an Excess Electron
- 15.12.05** **Dr. Yannick Carissan**
Overview of Recent Theoretical Chemistry Contributions to SFB 551
- 12.01.06** **Elena Kordel**
Ab-Initio-Berechnung molekularer Eigenschaften
- 19.01.06** **Dr. David P. Tew**
Cusps and Correlation Factors
- 26.01.06** **Dr. Paola Nava**
ECPs in Turbomole
- 02.02.06** **Markus K. Armbruster (INT/FZK)**
Zweikomponentige ECPs
- 09.02.06** **13:00 Uhr (Achtung! Geänderte Uhrzeit)**
Dr. Bernd Schimmelpfennig (INE/FZK)
Computational Actinide Chemistry Close to Experiment
- 16.02.06** **Dr. Christian Neiss (INT/FZK)**
Explicitly Correlated Coupled Cluster Response Theory