

# Seminar über Theoretische Chemie

jeweils donnerstags, 15:30 Uhr, im Seminarraum 408, 4. OG, Geb. 30.44

- 22.10.15** **Dr. Shachar Klaiman** (Universität Heidelberg)  
Barrierless single-electron-induced cis–trans isomerization
- 29.10.15** **Christian Lasar** (Universität Oldenburg)  
Explicitly correlated self-consistent-field theory
- 05.11.15** **Dr. Adam Kubas** (MPI für chemische Energiekonversion, Mülheim)  
Solid-state chemistry beyond DFT
- 13.11.15<sup>\*)</sup>** **Prof. Dr. Gustavo E. Scuseria** (Rice University, Houston, USA)  
Novel coupled-cluster approaches for strongly correlated electrons
- 03.12.15** **Prof. Dr. Ralph Jaquet** (Universität Siegen)  
Quantum reactive scattering at low collision energies and ro-vibrational bound states near the dissociation limit for the  $H_3^+$  system
- 10.12.15** **Dr. Peter Limacher**  
Seniority-zero wavefunctions: How to treat multireference problems with single-reference ansätze
- 14.01.16** **Dr. Michael Trumm** (Institut für Nukleare Entsorgung, KIT)  
Taking An(III)/Ln(III) partitioning to the next level
- 21.01.16** **Dr. Olaf Hübner** (Universität Heidelberg)  
Combined quantum-chemical and matrix-isolation study on  $V_2$  and VO:  
Excited electronic states
- 28.01.16** **Dr. Lies Broeckaert**  
Formation and functionalization of intermetalloid clusters

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

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<sup>\*)</sup> Freitag, den 13.11.2015, 15:30 Uhr, im Seminarraum 007, Erdgeschoss, Geb. 30.44