

# Seminar über Theoretische Chemie

jeweils donnerstags, 15:30 Uhr, im Seminarraum 408 (Geb. 30.44)

- 26.10.17**     **Yannick Franzke**  
Implementation of efficient analytical gradients within X2C
- 02.11.17**     **Dr. Uwe Huniar**  
COSMO-RS: Theory and applications
- 09.11.17**     **Dr. Peter Limacher**  
Seniority-Increasing Cluster Theory: A solution to all our multi-reference problems?
- 16.11.17**     **Dr. David Tew**  
Low scaling electronic structure theory
- 23.11.17**     **Fabian Mack**  
Calculation of chemical shielding constants with meta-GGA functionals
- 30.11.17**     **Dr. Jiří Chmela**  
Optical processes of molecules with rigid ligands: theory and experiment complementing
- 07.12.17**     **Dr. Stephan Kohaut**  
Cooperative effects in transition metal catalysis
- 18.01.18**     **Twinkle Yadav**  
Spin orbit coupling in transition metal compounds
- 25.01.18**     **Ansgar Pausch**  
Atoms and molecules in strong magnetic fields
- 01.02.18**     **Dr. David Sulzer**  
Tailoring the nitroxide exchange reaction to build organized polymer networks
- 08.02.18**     **Timo Schulz**  
Multireference perturbation theory