Special Topics in Theoretical Chemistry

Spring Semester 2013

Time: 13:15

Room: HCI J243

Name	Date	Topic
Ron Shepard	28.01	Invited Guest Speaker
	19.02	
Stefan Knecht	26.02	Theoretical Techniques for a Rational Description of Catalytic Activities and spectroscopy of Heavy-Element Compounds – Activation of Inert Molecules and Molecular Bonds with Rare-Earths
Pawel Tecmer	05.03	Towards Reliable (Quantum Chemical) Modeling of Lanthanide Complexes
Katharina Boguslawski	12.03	A Quantum Description of the Chemical Bond
Thomas Weymuth	19.03	Investigating Real-Life Transition Metal Reactions with Density Functional Theory
Halua Pinto de Magalhaes	26.03	Hypervalent Bonding of Late p-Block Elements: Reactivity of λ3-Iodanes
	02.04	Easter
Oliver Sala	09.04	Trifluoromethylation - MD and Meta-Dynamics
Arndt Finkelmann	16.04	QM/MM for Haptic Quantum Chemistry
Moritz Haag	23.04	Haptic Quantum Chemistry
Maike Bergeler	30.04	Transition State Search Methods
Marta Bruska Arseny Kovyrshin	07.05	Spectroscopic Signatures of Fe-S Clusters Oxidation Products Efficient and Selective Methods for Calculation of Excited-State Energies and Gradients in Extended Systems
Joël Gubler Martina Minges Minh Dao Denitsa Baykusheva	14.05	Calculation of Mössbauer Spectra of Resting State Models for the [Fe]-Hydrogenase Active Centre Investigating Carbene Ligands for Schrock-Type Dinitrogen-Fixation Catalysis Benchmark Calculations of Various Quantum Chemistry Programs Implementation of VCD Spectra Calculations with SNF/ADF
Benjamin Simmen	21.05	Progress on the Relativistic pre–BO Theory
Sebastian Keller	28.05	First applications of Maquis DMRG