Special Topics in Theoretical Chemistry

Autumn Semester 2013

Time: 13:30

Room: HCI G232

Name	Date	Topic
Markus Reiher	18.09	How to write a paper (at 13.00)
	25.09	
Tim Hangele	01.10	Relativistic pseudopotentials for superheavy elements (at 10.30)
	09.10	
Arndt Finkelmann	16.10	MM and QM/MM methodologies within the SAMSON program framework
Thomas Weymuth	23.10	Theoretical raman optical activity spectroscopy of protein β-Sheets
Johannes Hachmann	25.10	From high-throughput quantum chemistry to the rational design of organic semiconductors - a big data and materials informatics approach.
Stefan Knecht	30.10	Mössbauer spectroscopy for heavy atoms
Christian Schilling	06.11	Generalized Pauli constraints and their physical relevance
Christoph Jacob	06.11	Alles über PyADF (at 15.00)
Hitoshi Goto	13.11	Finding Minima-Conformations, Crystal Polymorphs, and Protein-Peptide Complexes
Florian Krausbeck	20.11	Potential Reconstruction based on DMRG spin densities
Moritz Haag	26.11	Molecular systems in virtual environments (at 16.45 HCI J3)
Martin Stiebritz	27.11	A role for FeS clusters in tRNA recognition?
	04.12	
Yingjin Ma	11.12	New quantum chemical methods based on the renormalization group
Benjamin Simmen	11.12	Progress on the RMFT
Paul Nicu	17.12	Calculations and interpretation of vibrational circular dichroism spectra
Stefan Jungen	18.12	Investigation of Trifluoromethylation Reaction Mechanisms
Prof. Celestino Agneli	18.12	Multireference Perturbation Theory: the n-electron valence state approach
Arseny Kovyrshin	18.12	Prospective Development of the Complete-Graph Tensor Network States