Special Topics in Theoretical Chemistry

Spring Semester 2014

Time: 13:30

Room: HCI G232

Name	Date	Topic
	19.02	no seminar
Markus Reiher	26.02	How to write a paper
Carmen Herrman	04.03 - 05.03	Molekulare Elektronik
Andrea Muolo	11.03	The simulation of ring-polymers: an introduction(at 13.00)
Arseny Kovyrshin	12.03	Prospective Development of the Complete-Graph Tensor Network States
	19.03	no seminar
	26.03	no seminar
Florian Krausbeck	02.04	Weitao Yang - Discovering His Life in 20 Minutes.
Oliver Sala Maike Bergeler	09.04 09.04	i) Solvent Modelling (PCM-based, Microsolvation and Cluster-Continuum) ii) Radical Reaction Mechanisms in Solution by ab-initio Molecular Dynamics. TS searches: procedures, pitfalls and possible solutions.
Sebastian Keller	16.04	DMRG, Maquis, etc...
	23.04	easter
Patrick Zobel	29.04	Relativistic Propagators and DFT Studies in Homogeneous Catalysis
Stefan Knecht	30.04	Multireference Perturbation Theory based on an DMRG wave function: latest developments
Benjamin Simmen	06.05	Pre-Born-Oppenheimer Theory with Explicitly Correlated Wave Functions (16.45 HCI J3)
Martin Stiebritz	14.05	A role for Fe4S4 clusters in tRNA recognition — A theoretical study.
Tom Penfold	20.05	Investigating the excited state dynamics of Cu(I)-phenanthrolines. (13.00 HCI J4)
Yingjin Ma	21.05	Gradients of a State-Average DMRG-SCF state
Halua Pinto de Magalhaes	28.05	Analysis of the Nature of Bonding of Hypervalent Iodine Compounds by the Methodology of Domain-averaged Fermi Holes
Emmanuel Fromager	06.08	Multiconfiguration DFT: separation of correlations in coordinate or configuration space ?
Stefano Battaglia	06.08	TBA