Special Topics in Theoretical Chemistry

Autumn Semester 2012

Time: 13:35

Room: HCI J243

Name	Date	Topic
Florian Krausbeck	16.10	Masterthesis: Implementation of a Solvation Model for Theoretical IR and VROA Spectroscopy
Katharina Boguslawski	23.10	Entanglement Measures and Electron Correlation Effects
Pawel Tecmer	30.10	The Electronic Spectrum of $CUONg_4$ (Ng = Ne, Ar, Kr, Xe): New Insights in the Interaction of the CUO Molecule with Noble Gas Matrices
Halua Pinto de Magalhaes	6.11	λ3-Iodane Based Functionalization of Arenes: a Mechanistic Study of the Reductive Elimination Step Revealing the Importance of the Hypervalent Bond
Arndt Finkelmann	6.11	How to perform a QM/MM calculation
Oliver Sala	20.11	Investigation of the Solvent Effect on two Competing Trifluoromethylation Reaction Mechanisms Involving λ3-Iodane Reagents
Maike Bergeler	27.11	Systematic Investigation of the Fe4S4-Cluster Reactivity Towards Reactive Oxygen Species
Moritz Haag	27.11	Real-Time Quantum Chemistry
Martin Stiebritz	4.12	The TS Flexibility Model
Sebastian Keller	4.12	DMRG in Quantum Chemistry and Condensed Matter Physics
Marta Bruska	11.12	Calculating NRVS spectra for FeFe Hydrogenases
Thomas Weymuth	11.12	Strategies and Methods in Inverse Quantum Chemistry
Benjamin Simmen	18.12	Progress on the Relativistic Many-1/2-Fermion Theory and the BlueBerry QC Engine
Daoling Peng	18.12	Local Relativistic Exact Decoupling