

# Special Topics in Theoretical Chemistry

Spring Semester 2012

Time: 13:15

Room: HCI J243

Name	Date	Topic
Anatole von Lilienfeld	17.01	From Electronic Structure Theory to Rational Compound Design
Michael Steinlechner	06.03	Locating Minimum Energy Crossing Points in Spin-Forbidden
Florian Krausbeck	06.03	Solvation Effects on the IR/Raman/ROA Spectra of Polypeptides
Daoling Peng	13.03	Progress in Relativistic Infinite-Order Decoupling Methods
Thomas Weymuth	20.03	Heavy Metal: A Challenge for Density Functionals
Moritz Haag	27.03	HQC Work in Grenoble
Katharina Boguslawsky	03.04	Accurate Ab Initio Spin Densities
This talk will be held in the LPC PC-Colloquium. Time: 16.45 Room: HCI J3		
	10.04	easter - no seminar
Martin Stiebritz	17.04	The TS Flexibility Model
Arndt Finkelmann	24.04	QM/MM for Haptic Quantum Chemistry? Problems which Need to be Solved
	01.05	labour day - no seminar
Marta Bruska	07.05	A Multi-Strategy Tool for Transition State Search
Halua Pinto de Magalhaes	14.05	Reactivity and Electronic Structure of Hypervalent $\lambda^3$ -Iodanes: the Role of the 3-center-4-electron Bond
Hans Peter Lüthi	14.05	TURBOMOLE-XML-eXist, An Infrastructure for the Generation, Analysis and Exchange of Quantum Chemical Data
Maike Bergeler	21.05	X-ray Absorption Spectroscopy: A Tool for the Analysis of 4Fe-4S Cluster
Benjamin Simmen	28.05	A Relativistic Many 1/2-Fermion Theory
Pawel Tecmer	28.05	Electronic Spectroscopy of Uranium-Containing Complexes