

FS 2010

Seminar Special Topics in Theoretical Chemistry FS2010

Time: Wednesdays 01:00 p.m.

Room: HCI J 243

Date	Name	Topic	Exceptions
17.02.	Claudio Greco	QM/MM studies in electron transfer events triggered by substrate binding in [FeFe]-hydrogenase	
24.02.	Stefan Knecht	Parallel Relativistic Multiconfiguration Methods: New Powerful Tools for Heavy-Element Electronic-Structure Studies	The seminar will take place this week at 15.00 h, exceptionally
10.03.	no seminar		
17.03.	Edit	Solution of the Schrödinger equation without the introduction of the Born-Oppenheimer approximation	
24.03.	Villö	NMR Part III: The foundations of quantum chemical calculations of NMR parameter	
31.03.	no seminar		
07.04.	no seminar		
14.04.	Koni	Introduction to Parallel Programming: Thinking Parallel	
21.04.	Martin	Parallel Programming with MPI	
28.04.	Katharina	OpenMP	
05.05.	Koni	Parallel Scientific Computing: Boost::Threads/TBB in C++	
12.05.	Steven	Pd-Catalyzed Direct Carboxylation of Aryl Bromides with CO ₂ : Computational Investigations into Competing Mechanistic Pathways	
19.05.	Maren	Challenges in Density Functional Theory Part 1: Theoretical Foundations	
26.05.	Arndt, Moritz	Semesterarbeiten	
09.06.	Nicolas, Benjamin,	Semesterarbeiten	

	Maïke, Maxime		
26.08. Thursday	Daniel Rohr	Short-range DFT and long-range DMFT	The talk will take place in room HCI E2 and start at 15:00 h