

# Seminar Theoretical Chemistry

Spring 2011

time: Wednesdays 02:00 p.m.

room: HCI J 243

Date	Name	Topic/Title
09.03.	Steven, Villö	New computer facilities
22.03. (Tue@15:00) HCI D4	Ralph Koitz, TU München	Scalable properties and magnetic features of palladium clusters
23.03.	Moritz, Arndt	Master thesis
30.03.	Edit	Non-BO theory
05.04. (Tue@15:00) HCI H2.1	Thomas	2D-IR spectroscopy
13.04.	Dr. Daoling Peng	Towards exact decoupling of the Dirac Hamiltonian, the relativistic two-component methods
20.04.	Steven	N <sub>2</sub> fixation
27.04.	Easter	
04.05.	Marta	Hydrogenase/TS search
11.05.	no seminar	
18.05.	no seminar	
25.05. @11:00 HCI G 3	Dr. Sebastian Kozuch, The Weizmann Institute of Science, Israel	What Makes for a Good Catalytic Cycle? Insights from the Energetic Span Model
31.05. (Tue@13:00) HCI J243	Katharina	Advances in DMRG