6th C4 Workshop

05 June 2019

University of Zurich, Irchel Campus

Lecture Hall Y03-G-85

Program

Time	Topic	Speaker
09:45 - 10:30	Revealing molecular secrets with theoretical beamlines	Sonia Coriani, TU Denmark
10:30 - 11:15	Exchange-correlation functionals from the strong-coupling limit of density functional theory	Paola Gori-Giorgi, VU Amsterdam
11:15 - 11:35	DMRG for Vibrational Spectroscopy	Alberto Baiardi, ETH Zurich
11:35 - 11:55	Using I=1 to improve nonadiabatic dynamics	Max Saller, ETH Zurich
12:00 - 13:00	*Lunch Break*	
13:00 - 13:45	QM/MM in material sciences - solid-state interfaces and absolute standard electrode potentials	Thomas Hofer, University of Innsbruck
13:45 - 14:30	Fully Atomistic Embedding Approaches for the Computational Spectroscopy of Complex Systems: Status and Perspectives	Chiara Cappelli, Scuola Normale Superiore, Pisa
14:30 - 14:50	Gaussian and Plane Waves Implementations of the Density Functional Embedding Theory	Vladimir Rybkin, University of Zurich
14:50 - 15:10	On-surface synthesis and characterization of antiaromatic and open-shell indeno[2,1-b]fluorene polymers	Kristjan Eimre, EMPA
15:15 - 15:45	*Coffee Break*	
15:45 - 16:30	Chemical space for small molecules and beyond	Jean-Louis Reymond, University of Bern
16:30 - 16:50	IBM RXN for Chemistry: Predicting Chemical Reactivity using the Molecular Transformer	Philippe Schwaller, IBM
16:50 - 17:10	The Chemoton Project for Chemical Reaction Space Exploration	Jan Unsleber, ETH Zurich