ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

COMPETENCE CENTER FOR COMPUTATIONAL CHEMISTRY C4

ETH Zürich / University of Zürich / IBM Research

Seminar Programm Herbstsemester 2014

Auditorium HCI J7, ETH Hönggerberg

13:00-14:00

24. 10. 2014 (*jointly with the Seminar on Theoretical Chemistry, Molecular Spectroscopy and Dynamics*) *
Prof. Dr. Rollin King, Bethel University, St. Paul, Minnesota (USA)
Optimizing the Optimizer: Practically Locating Interesting but Challenging PES Minima

06.11. 2014
Dr. Ivano Tavernelli, EPF Lausanne / IBM Research, Zürich
TDDFT-based Nonadiabatic Dynamics with Relativistic Effects

10. 11. 2014 (*Seminar of the Laboratorium für Organische Chemie*) **
Prof. Dr. Frank Neese, MPI for Chemical Energy Conversion, Mülheim/Ruhr (D)
Accurate ab initio Quantum Chemistry for Large Molecules. New Developments and Future Opportunities

13. 11. 2014
Dr. Gregory Landrum , Novartis Institutes for Biomedical Research, Basel (CH)
The Interpretability Dilemma: Making Models Useful

27.11. 2014
Prof. Dr. Claudia Draxl, Humboldt-Universität zu Berlin, Berlin (D) ***
Theoretical spectroscopy: Concepts and challenges for novel functional materials

11.12.2014
Prof. Dr. Ville R. I. Kaila, Technische Universität München, München (D)
Multi-scale Molecular Simulations on Biological Energy Conversion

*) Auditorium HCI J6, 16:15 (note that the seminar is on a Friday)
**) Auditorium HCI J3, 16:00 (note that the seminar is on a Monday)
***) Joint invitation with the Institute for Theoretical Physics

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