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 2012

Auditorium HCI J6, ETH Hönggerberg
13:00-14:00 (unless otherwise noticed)

16. 10. 2012 (*hosted by ETH Zürich Kolloquium für Physikalische Chemie*)
Prof. Christoph van Wüllen TU Kaiserslautern (Deutschland)
Zero field splitting of multinuclear transition metal complexes: a challenge for density functional methods

01. 11. 2012 (*seminar starts at 12:00 in auditorium HCI J6*)
Dr. Lorna Smith, University of Oxford, Oxford (UK)
Ligand binding and protein misfolding: new insights from MD simulations.

08.11. 2012
Prof. Thomas F. Miller III, California Institute of Technology, Pasadena (CA, USA)
Title open

22. 11. 2012 (*hosted by University of Zürich Institute of Physical Chemistry Seminar*)
Prof. Alessandro Laio, Intl. School for Advanced Studies, SISSA, Trieste (Italy)
Exploring the universe of protein structures by atomistic simulations: beyond the Protein Data Bank

03.12. 2012 *(Note that 3.12.2012 is a Monday; seminar takes place in HCI J7 at 15:00)*
Dr. Setphane Redon, INRIA Grenoble Rhône-Alpes, Saint Ismier (France)
Theory and algorithms for adaptive particle simulations

13. 12. 2012 (*hosted by University of Zürich Institute of Physical Chemistry Seminar*)
Dr. Damien Laage, École Normale Supérieure, Paris (France)
Towards a microscopic picture of protein hydration dynamics

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