

COMPETENCE CENTER FOR COMPUTATIONAL CHEMISTRY C4
ETH Zürich / University of Zürich / IBM Research**Seminar Programm Frühjahrssemester 2009**Auditorium HCI J7, ETH Hönggerberg
13:00-14:00

26. 02. 2009

Thomas Schulthess, Swiss Center for Scientific Computing (Manno, Schweiz)
Intricacies of Electronic Structure and Many-Body Simulations in the Cuprate High-Temperature Superconductors

12. 03. 2009

Thomas Hofer, ETH Zürich /Universität Innsbruck (Innsbruck, Österreich)
Electronic Quantum Effects in Molecular Simulations - Applications of QM/MM Models in Solution Chemistry

26. 03. 2009

Giovanni Ciccotti, University of Rome, La Sapienza (Rome, Italy)
Minimum Free Energy Paths: the Case of the Nucleation Path in the Two-Dimensional Ising Model

09. 04. 2009

Chris Mundy, Pacific Northwest National Laboratory (Richland, WA, USA)
Back to the Future: Parameterizations of First-principles Interaction Potentials for Probing the Statistical Mechanics of Hydrogen Bonded Fluids

23. 04. 2009

Benoit Roux, University of Chicago (Chicago, IL, USA)
Multiscale Approach to the Activation/Inactivation of Src Kinases

07. 05. 2009

Barbara Kirchner, Universität Leipzig (Leipzig, Deutschland)
Ionic Liquids from Theoretical Calculations

14. 05. 2009

Gustavo Scuseria, Rice University (Houston, TX, USA)
Screened Hybrid Functionals for Solid-state Chemistry and Physics

28. 05. 2009

Daan Frenkel, Cambridge University (Cambridge, United Kingdom)
Entropy, Disorder and Packing