

**COMPETENCE CENTER FOR COMPUTATIONAL CHEMISTRY C4**  
**ETH Zürich / University of Zürich / IBM Research****Seminar Programm Frühjahrssemester 2012**Auditorium HCI J7, ETH Hönggerberg  
13:00-14:00

01. 03. 2012

**Prof. Núria López**, Institut Català d'Investigació Química, Tarragona (Spain)  
Selectivity in Hydrogenation Reactions: the Role of Theoretical Simulations

15. 03. 2012

**Prof. Dr. Patrick Bultinck**, Ghent University, Ghent (Belgium)  
The Fukui matrix, an algebraic tool for the understanding of Fukui functions, their magnitude and sign and effects of correlation and degeneracy

12. 04. 2012 Easter Break (no seminar)

26. 04. 2012

**Dr. Hans Martin Senn**, Lecturer, University of Glasgow, Glasgow, Scotland (UK)  
Insights into enzymatic catalysis using computational chemistry:  
From docking to coupled-cluster methods.

03. 05. 2012

**Prof. Alán Aspuru-Guzik**, Harvard University, Cambridge, MA (USA)  
Finding renewable energy materials using one screensaver at a time:  
The Harvard Clean Energy Project

10. 05. 2012

**Dr. Saron Catak**, Center for Molecular Modeling, Ghent University, Zwijnaarde, (Belgium)  
First principles metadynamics simulations of 'Rare Events' in biological systems

24. 05. 2012

**Prof. Tim Clark**, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen (Germany)  
Simulating soft electronic devices:  
High-performance NDDO calculations for new materials