

ACMM Spring Symposium 2012

We are happy to announce that the Spring Symposium of the Amsterdam Center for Multiscale Modeling (ACMM) will take place on *Thursday 28 June 2012*.

We have invited a number of internationally renowned speakers, who will give lectures on several aspects of Multiscale Modeling, ranging from physical chemistry to biology. There is no registration fee and the symposium is open to computational scientists, students, and anyone else with an interest in the ACMM.

When: Thursday, 28 June 2012, 11.00 - 17.30

Where: PC Hooft Huis, Spuistraat 134, 1012 VB Amsterdam ([location map](#))

The program is as follows:

11.00 Coffee

11.20 **Maxim Fedorov, University of Strathclyde**

Theory of Molecular Liquids & Computational Biomolecular Design:
predicting the solvation behaviour of drug-like molecules and pollutants

12.10 **Herma Cuppen, Radboud University Nijmegen**

Long-timescale simulations of diffusion in molecular solids

13.00 Lunch

14.00 **David Swendson, University of Amsterdam**

A Classical Model for Nonequilibrium Quantum Transport: The Dynamics
for Classically Mapped Fermions Method

14.40 **Oleg Gritsenko, VU University Amsterdam**

New developments in Density Matrix Functional Theory

15.20 Tea Break

15.50 **Davide Branduardi, MPI Biophysics, Frankfurt**

Understanding conformational transitions through string method: the
ATP-Mg case

16.40 **Laura Orian, University of Padova**

Rh(I) half-sandwich complexes: an insight into their structure and
catalytic activity in [2+2+2] cycloadditions of alkynes through Density
Functional Theory calculations

17.30 Closing followed by drinks