



# cecam *Da*CAM

Vienna, September 14, 2012

Danube Center for Atomistic Modelling



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TECHNISCHE  
UNIVERSITÄT  
WIEN  
Vienna University of Technology



CENTER FOR  
COMPUTATIONAL  
MATERIALS  
SCIENCE





## Opening of the Danube Center for Atomistic Modeling

**Venue:** Kuppelsaal  
Vienna University of Technology  
Karlsplatz 13  
A-1040 Vienna, Austria

**Date:** September 14, 2012

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participation and buffet dinner:  
R.S.V.P. until September 5, 2012 via email  
([gerhard.kahl@tuwien.ac.at](mailto:gerhard.kahl@tuwien.ac.at))



# Program

## 13:30 Welcome

Gerhard Kahl (Vienna University of Technology)  
Director of the DaCAM-Node (Vienna)

Susanne Weigelin-Schwiedrzik (University of Vienna)  
Vice-Rector of the University of Vienna

Johannes Fröhlich (Vienna University of Technology)  
Vice-Rector of the Vienna University of Technology

Georg Haberhauer (University of Natural Resources and Life Sciences, Vienna)  
Vice-Rector of the University of Natural Resources and Life Sciences, Vienna

Peter Mohn (Vienna University of Technology)  
President of the Center for Computational Materials Science (Vienna)

Dominic J. Tildesley (Unilever, UK)  
Director-elect of CECAM

Christoph Dellago (University of Vienna)  
Vice-President of the CECAM Council

## 14:15 Scientific contributions

14:15 Wilfred F. van Gunsteren (ETH Zürich)  
Biomolecular simulation: CECAM 1976, CECAM 2012, CECAM 2048

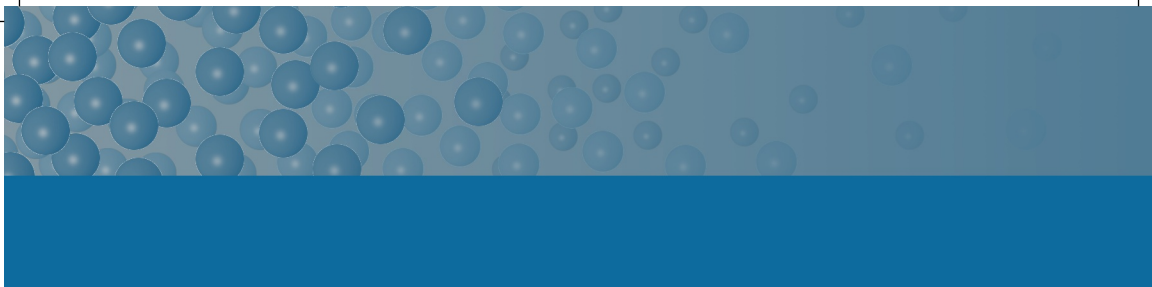
## 15:05 Coffee Break

15:35 Kurt Binder (JGU Mainz)  
Phase behavior of polymer-containing systems:  
recent advances by computer simulation

16:25 Jürgen Kübler (Darmstadt)  
Challenges in superconductivity and magnetism

## 17:15 End of the program

18:30 Buffet dinner



**CECAM (Centre Européen de Calcul Atomique et Moléculaire)**, founded more than 50 years ago, is a European organization devoted to the promotion of fundamental research on advanced computational methods and to their application to important problems in frontier areas of science and technology. The focus of the CECAM activities is on atomistic and molecular simulations in physics, materials science, chemistry and biology. CECAM activities range from the organization of scientific workshops to that of specific tutorials at the graduate level, from brain-storming meetings on timely topics to collaborative research projects, and sponsoring of an interesting visitors program as well as of specialized courses in computational sciences also at the master level. CECAM, with its headquarters hosted at the École Polytechnique Fédérale de Lausanne (Switzerland), has a nodal structure with currently 14 nodes all over Europe.



**DaCAM (Danube Center for Atomistic Modeling)** is the Austrian node of CECAM. Based in Vienna, it is run by the University of Vienna, the Vienna University of Technology, the University of Natural Resources and Life Sciences, Vienna, and the Center for Computational Materials Science (CMS), the latter one being the Austrian representative in the CECAM organization. The installation of a CECAM node in Vienna reflects both the long tradition as well as the strong scientific activities in atomistic and molecular simulations in the Vienna area: at the involved institutions, research in the field of atomistic and molecular simulations covers a wide spectrum of topics, ranging from solid state systems over soft matter systems to the field of biomolecular simulations. With the planned scientific activities, DaCAM aims to attract scientists from all over the world and to foster a mutually fruitful exchange of ideas. The geographical location of the DaCAM node offers an ideal opportunity to establish and to re-enforce contacts in the field of atomistic and molecular simulations to scientific groups in the neighbouring central and Eastern-European countries.

