

TERATEC - Paris June 2013

CECAM-the Simulation and Modelling of Atoms and Molecules in Europe

Dominic Tildesley CECAM and EPFL



History of CECAM

- The laboratory was founded in 1968 by Dr. Carl Moser, an American scientist naturalized in France
- 1969-1992: Orsay, Paris Sud
- 1992-2008: Ecole Normale Supérieure de Lyon
- 2008-2013 EPFL Lausanne Switzerland



Dr. Carl Moser, Director of CECAM
(Centre Européen des Calculs Atomiques
et Moléculaires), in his office in Orsay.
With Joey, Uxel and Johnnie Walker. July 1977.

copyright A.Olson, 2001

Core areas for CECAM

- Electronic Structure calculation
- Density Functional Theory
- Classical and quantum Monte Carlo
- Molecular dynamics
- First principles dynamics
- Coarse-grained simulation methods
- Computational Fluid dynamics
- Multi-scale modelling

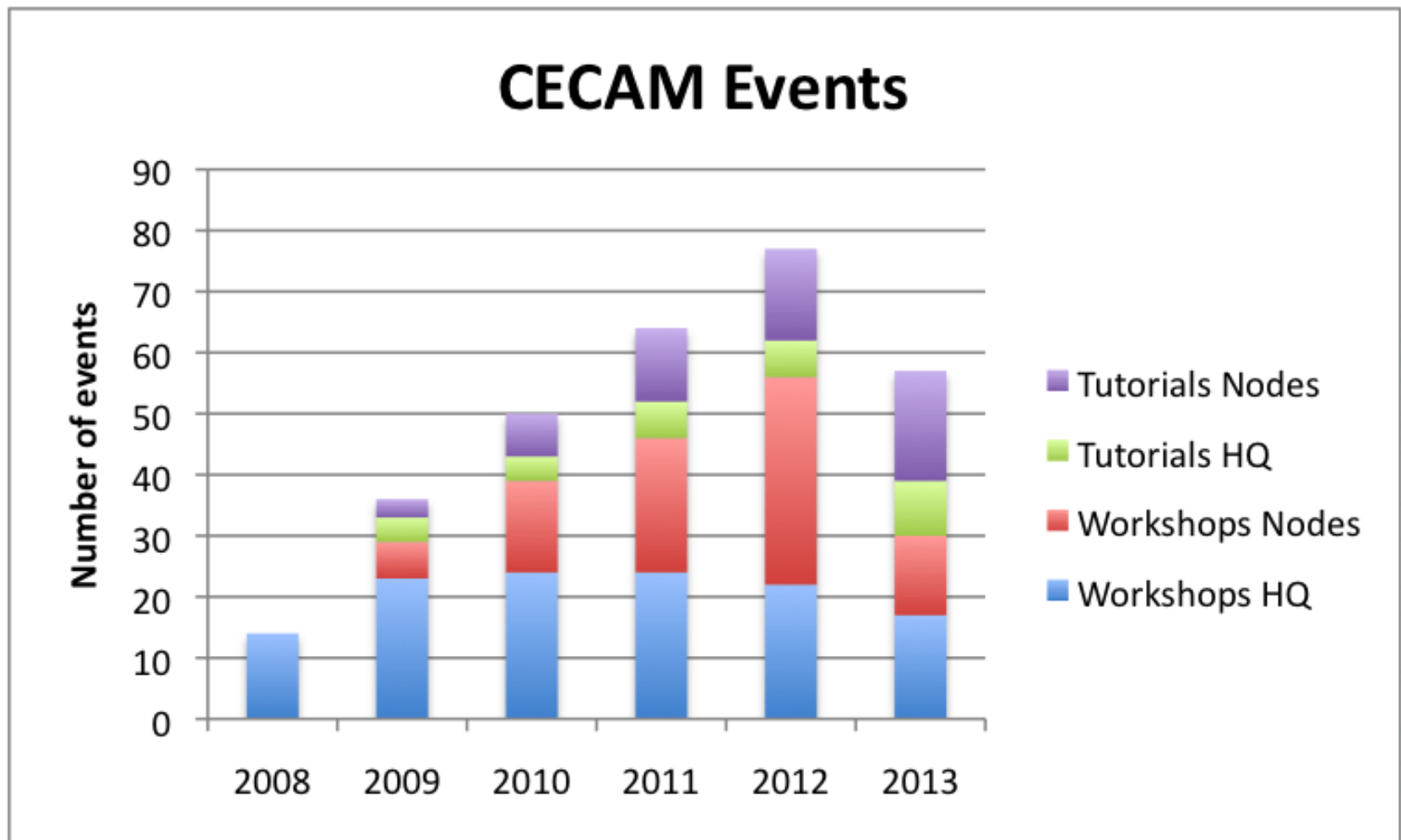
Events in 2012

- **Numbers**

- 54 workshops in total (22 in Switzerland, 34 in all of the nodes)
- 21 tutorials in total (6 in Switzerland, 15 in the nodes)
- See CECAM website for
 - details of all events
 - lists of participants
 - final recommendations



Number of CECAM events



Calculation of optical properties from first principles

Location : CECAM-HQ-EPFL, Lausanne, Switzerland

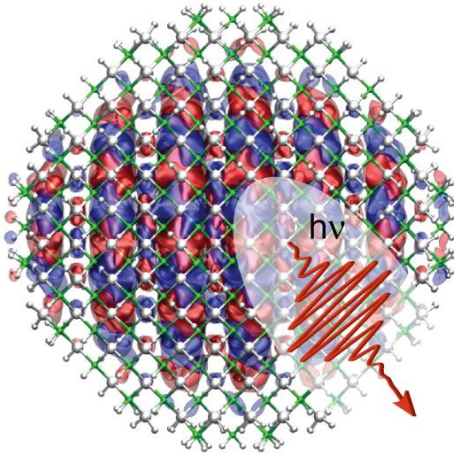
February 19, 2013 - February 22, 2013

Gabriel Bester:
Friedhelm Bechstedt
Claudia Draxl

Max Planck Institute for Solid State Research, Stuttgart, Germany

University of Jena, Germany

Humboldt-Universität Berlin, Germany



- Workshop considered optical properties and hence two-particle excitations such as excitons, which is at the frontier of today's ab-initio approaches.
- The structures are non- periodic along at least one of the dimensions calling for the treatment of large simulation cells with many-atoms.



Hermes 2012 tutorial

Hermes 2012
Summer School

Location : Cumberland Lodge, The Great Park, Windsor,
Berkshire, United Kingdom

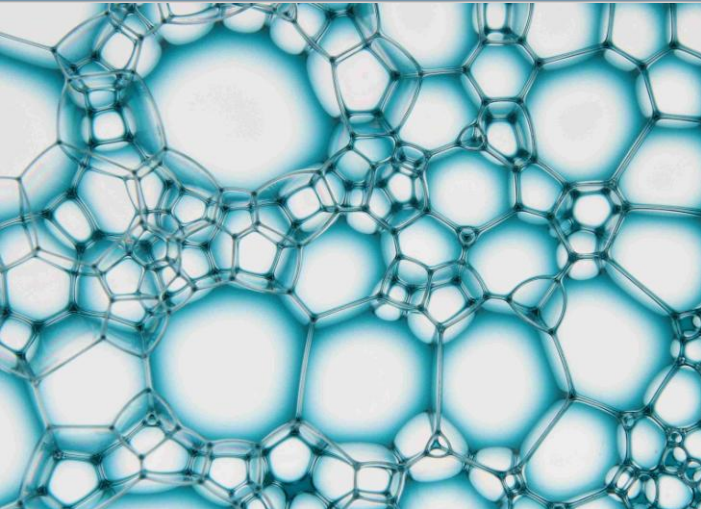
July 27, 2012 - July 30, 2012

- Jassel Majeবাদia ICSTM
- Massimo Riello Kings
- Al-Moatasem El-Sayed UCL
- Aeneas Wiener ICSTM
- Fabian Renn ICSTM
- Niccolo Corsini ICSTM
- Joseph Fallon ICSTM
- Eva Zarkadoula Queen Mary
- Tom Swinburne ICSTM

Craig Carter (MIT)
Vaclav Vitek (UPenn)
Helena van Swygenhoven (EPFL)



Dissipative Rheology of Foams



Location : Trinity College Dublin, Ireland

January 9, 2012 - January 12, 2012

Simon Cox

Aberystwyth University, UK

Isabelle Cantat

Université Rennes I, FR

Reinhard Hohler

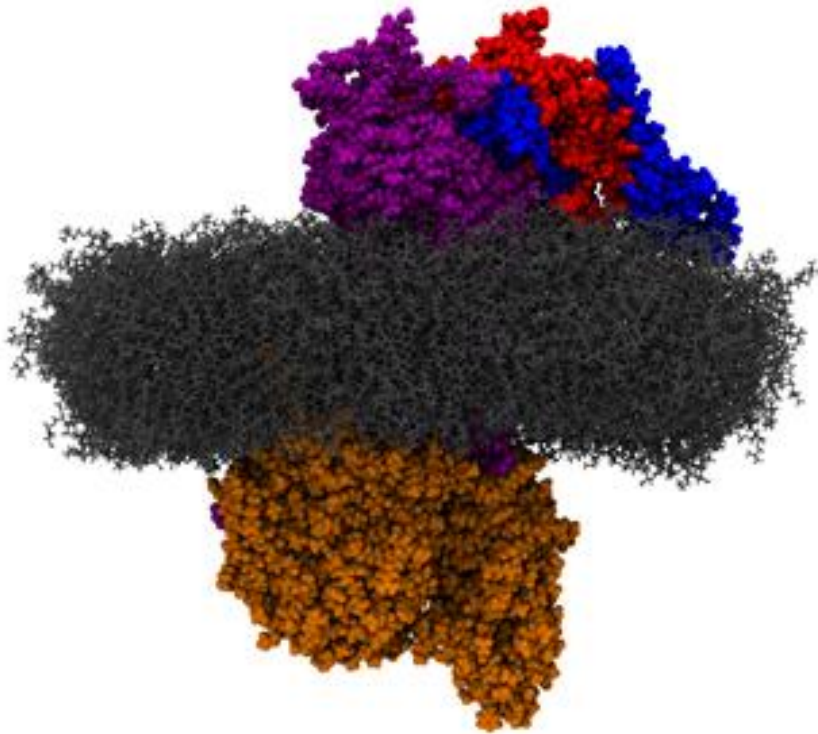
Université Paris-Est, Marne-la-Vallée, FR

Stefan Hutzler

Trinity College Dublin, IRE

- Many sources of dissipation within a flowing foam or emulsion have been described. They include viscous effects from the bulk and surfaces, interfacial rheology and the motion of surfactant molecules. Our goal is to develop computationally-efficient multi-scale methods that accurately represent these processes.
- Current effort is directed at developing bubble-scale models to predict a foam's rheological response.
- Durian's bubble model for the wet limit;
- Surface Evolver and vertex models for the dry, quasi-static regime;
- hydrodynamical models that include fluid flow in the interstices between the bubbles.

Molecular Simulation of Membranes Proteins



CECAM-HQ-EPFL, Lausanne, CH

March 7-9 2012

Ursula Roethlisberger EPFL CH

Mauro Boero University of Strasbourg , FR

Paolo Carloni German Research School
for Simulation Sciences, DR

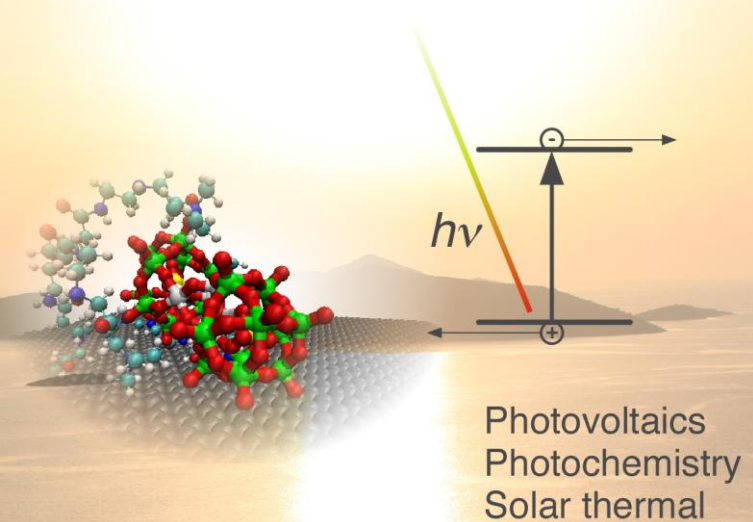
Ion transport and signaling processes are governed by membrane proteins, which allow cells to communicate with their surrounding environment. They determine whether or not the immune system is able to recognize a foreign cell. Membrane proteins are also responsible for cell adhesion in the tissues formation processes. They control a wide spectrum of metabolic processes, ion transfer in channels, and photosynthesis.

The CECAM Conference

Energy from the Sun

Computational Chemists and Physicists Take up the Challenge

September 10-14 2012 - Chia Laguna - Sardinia - ITALY



Cagliari Italy September 2012

- Energy from the Sun: Computational Chemists take up the Challenge

- 90 participants
- 8 themed sessions, 40 posters

The goal of this CECAM conference is to bring together computational chemists, physicists, and materials scientists who are addressing the problem of solar energy conversion and storage, from different perspectives. The focus will be on novel materials as well as on fundamental physical and chemical processes that control solar energy harnessing. Areas of interest include photovoltaics, photochemistry, photocatalysis, and solar to thermal conversion.

Some Research at CECAM

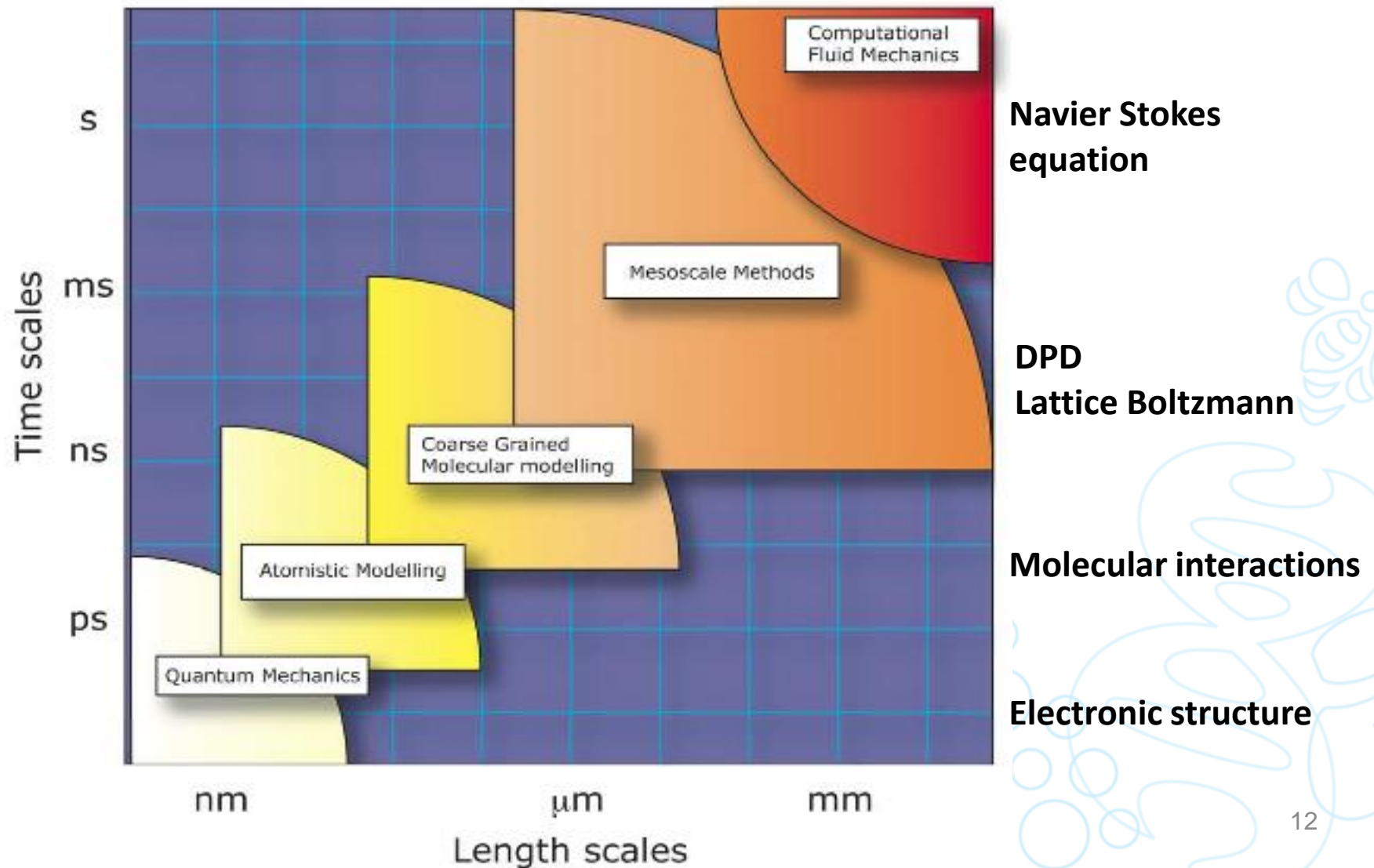
The Effect of Charge on Boundary Layer Lubrication

Patrice Malfreyt
Dominic Tildesley

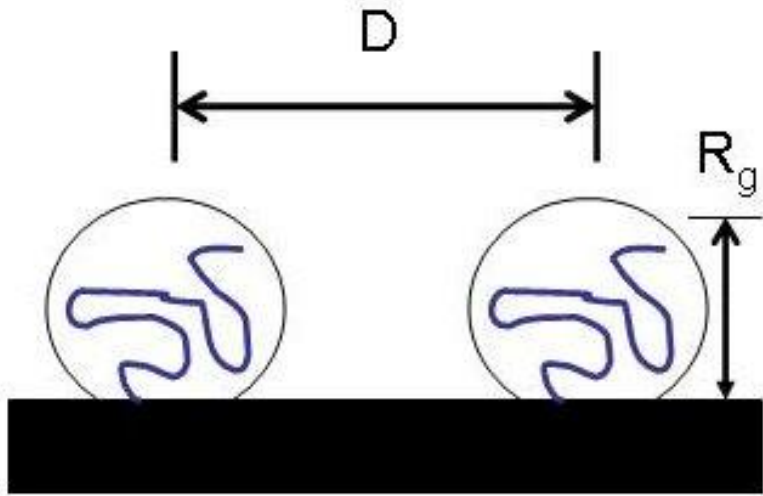
Clermont Ferrand
CECAM EPFL, Unilever



Multi-scale Modelling



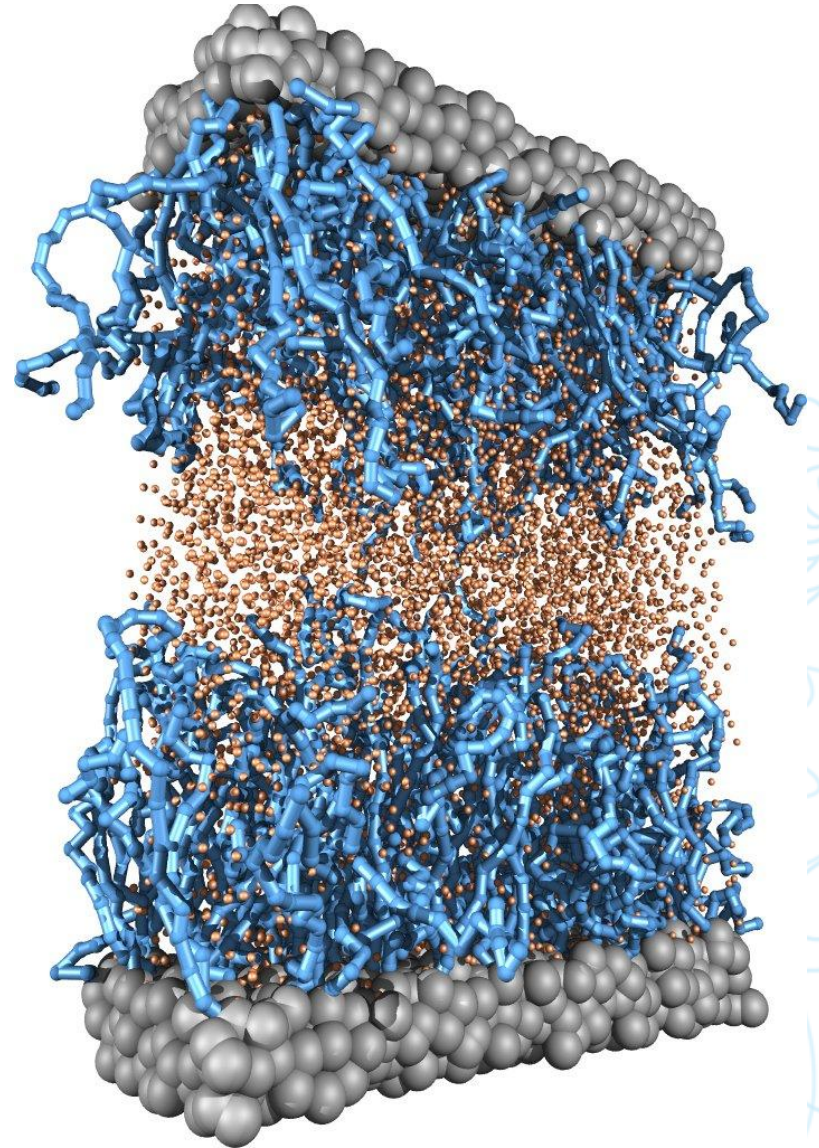
Simulation of Polymer brushes



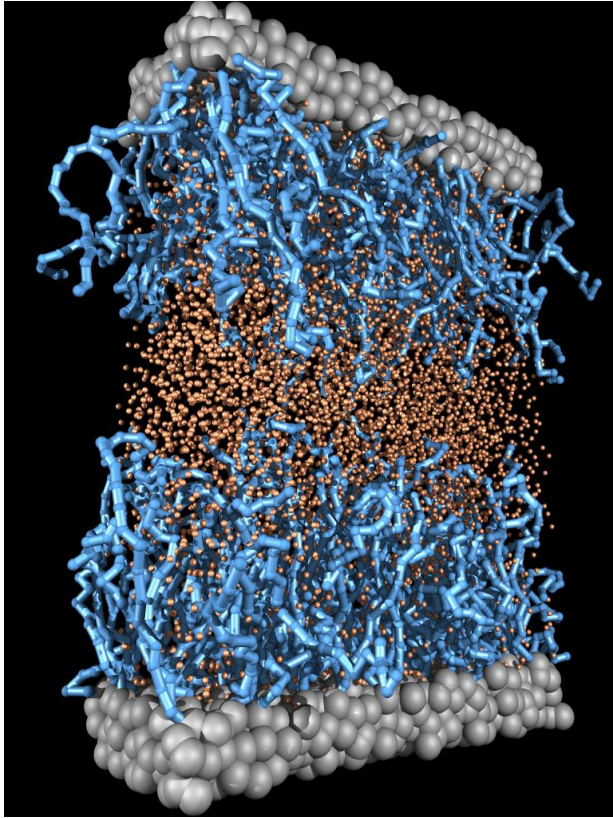
Polymer mushroom

The excluded volume repulsion (in a good solvent) balances the elastic pressure

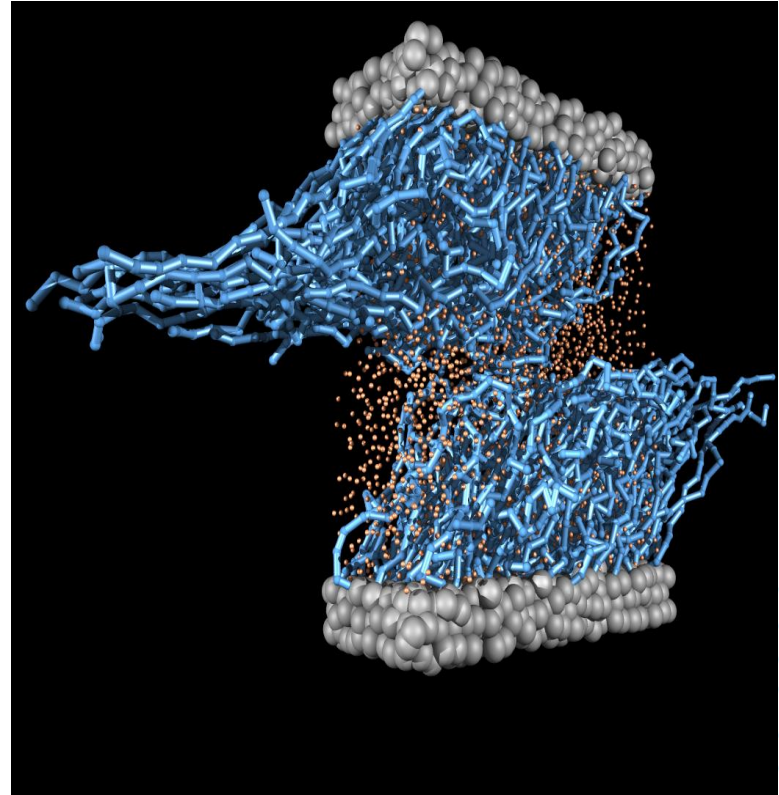
Alexander, de Gennes 1977



Neutral polymer brushes

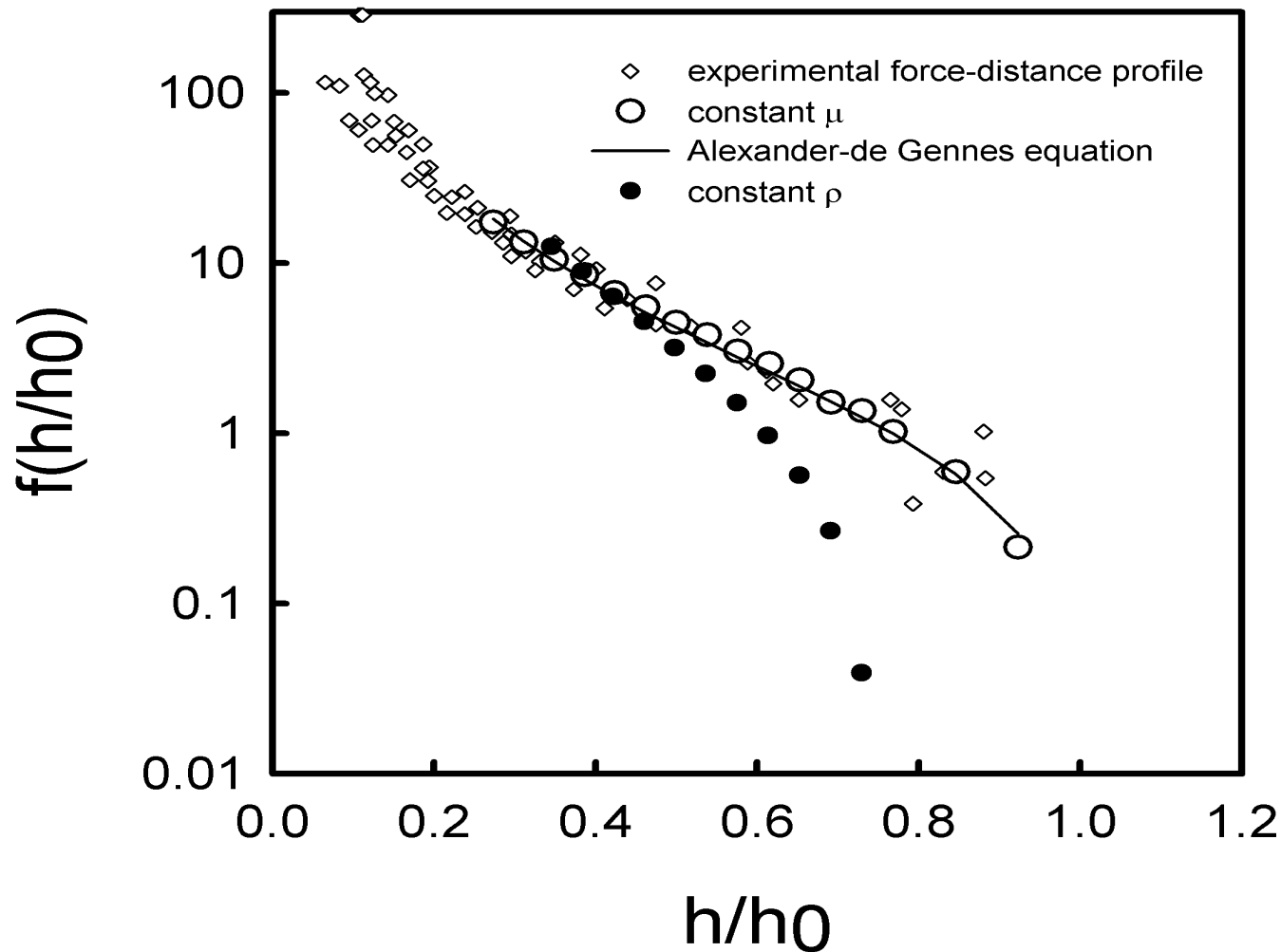


At equilibrium

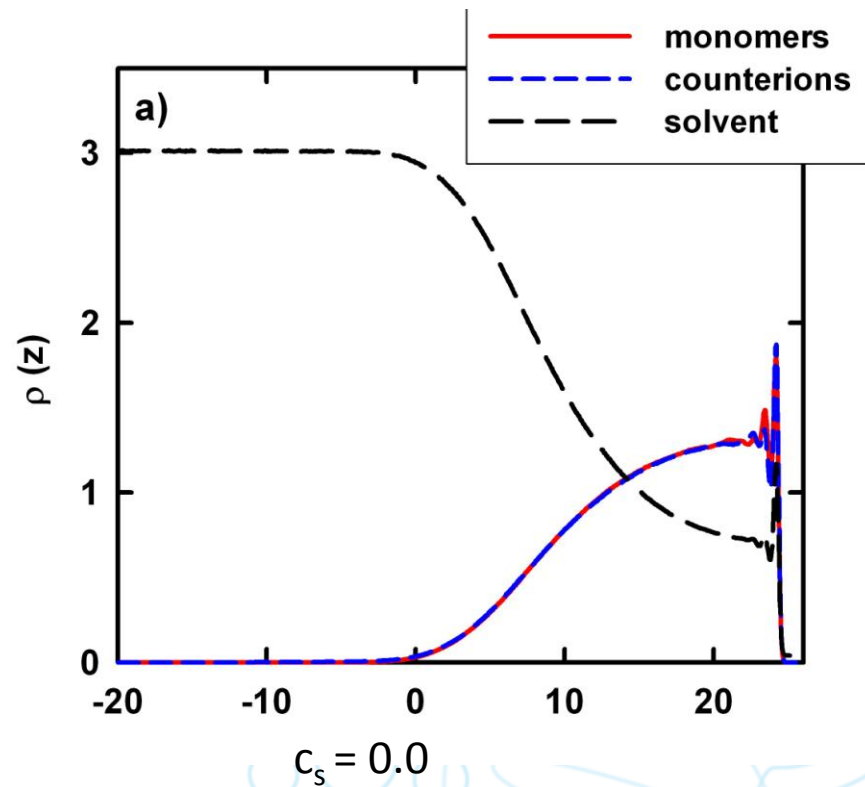
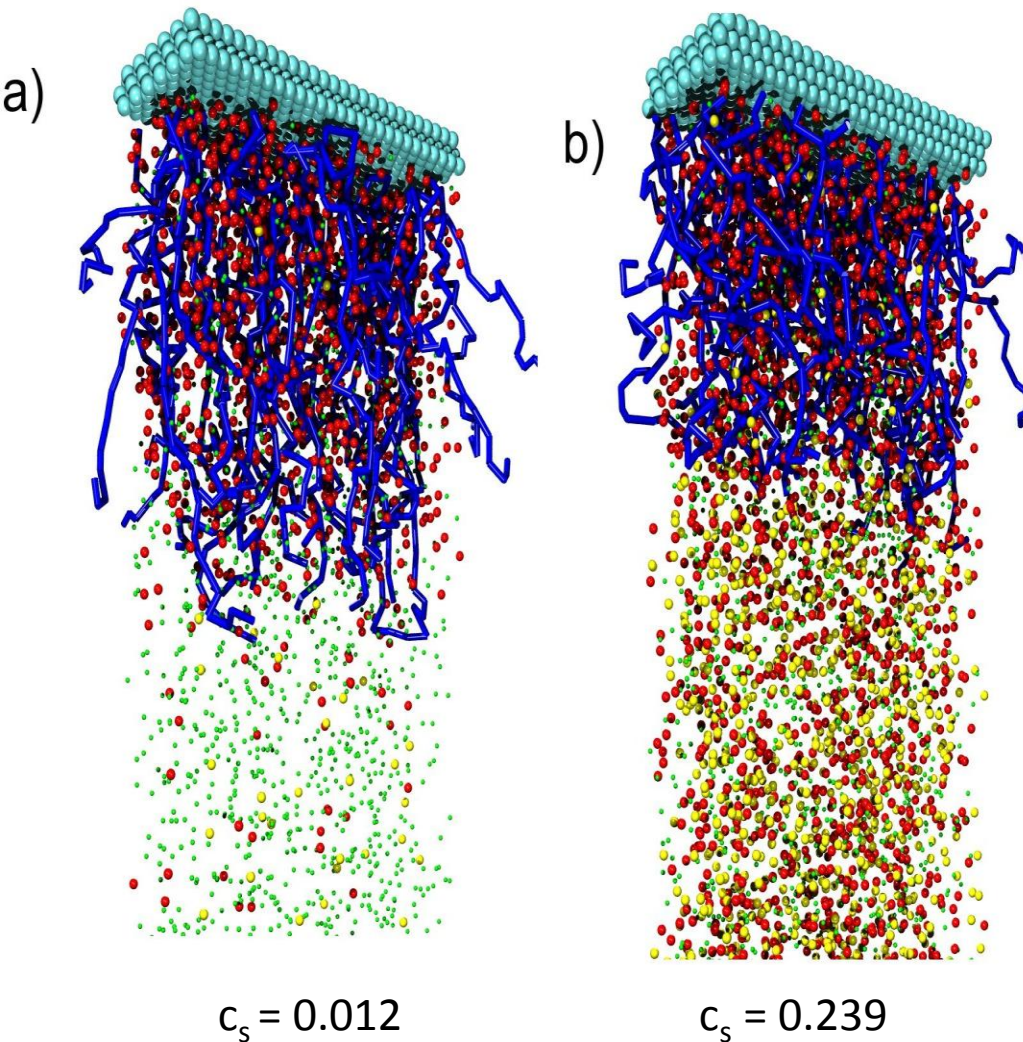


Under shear

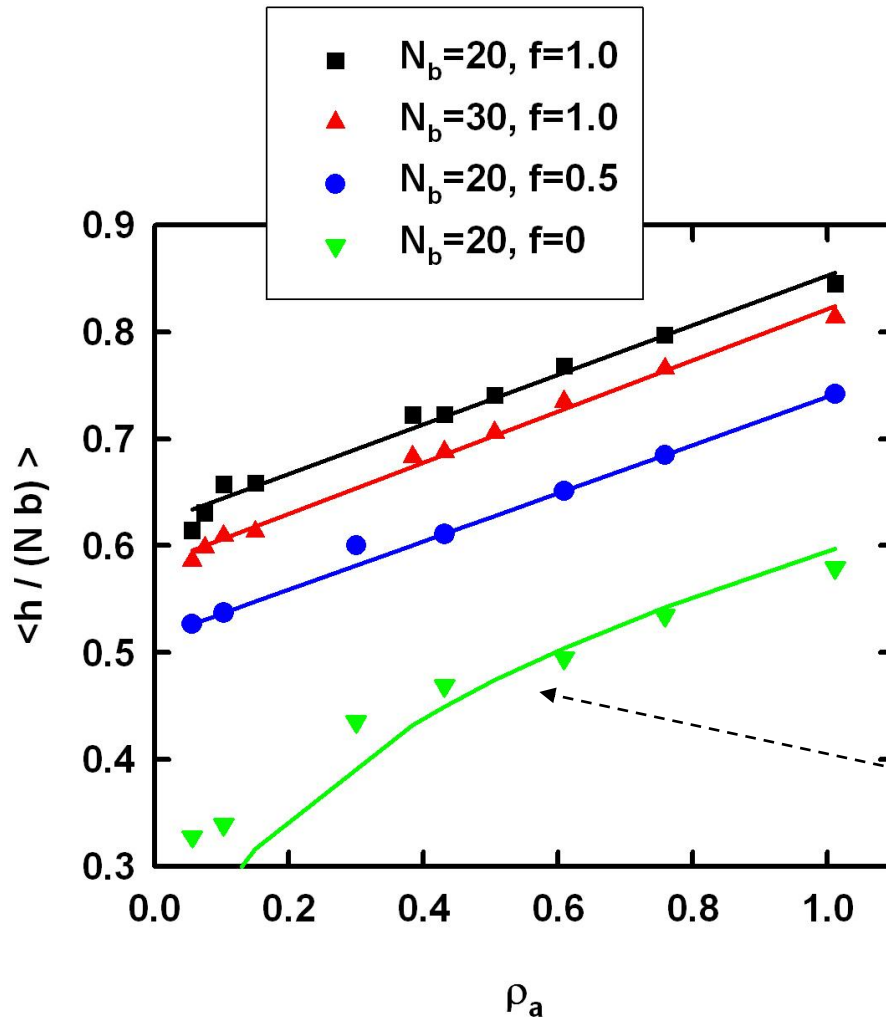
Force-distance curve for neutral polymer brushes



Modelling of polyelectrolytes single brush



Height of brush with grafting density



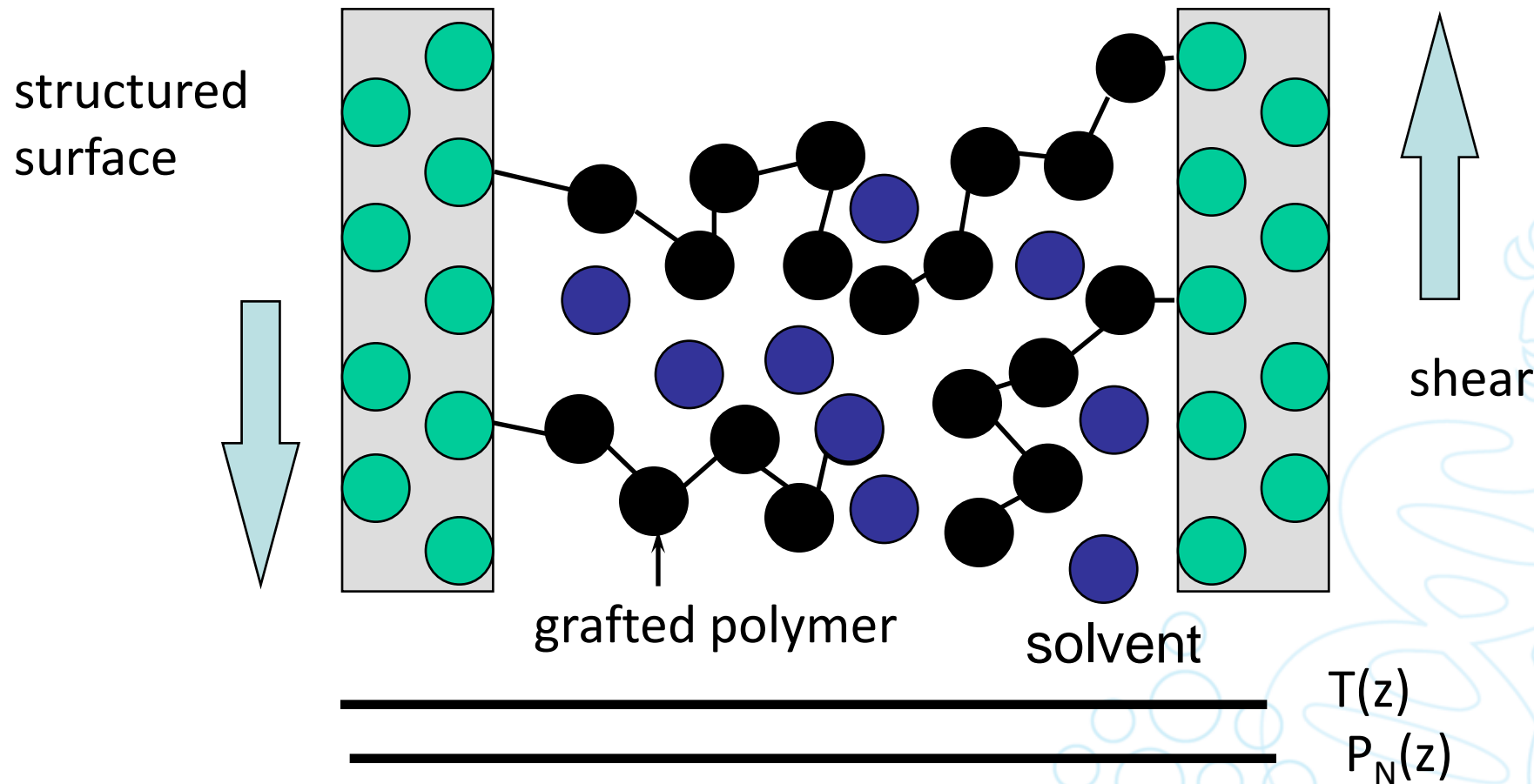
Charged brush

$$\frac{h}{N_b b} \simeq \frac{f + d^2 \rho_a}{1 + f}$$

Neutral brush

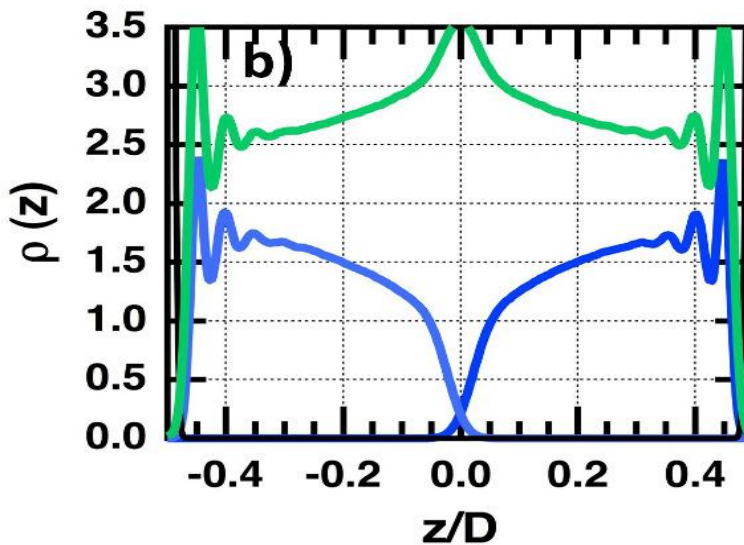
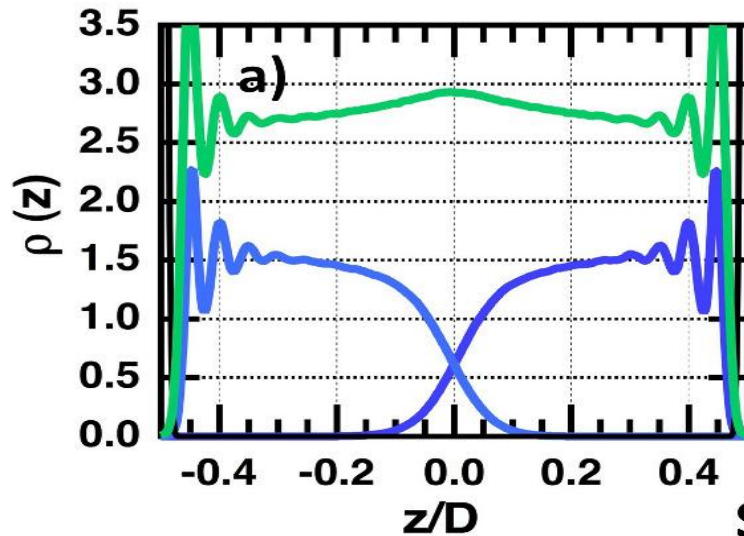
$$\frac{h}{(N_b b)} \approx \rho_a^{1/3}$$

The simulation of grafted polymers under shear



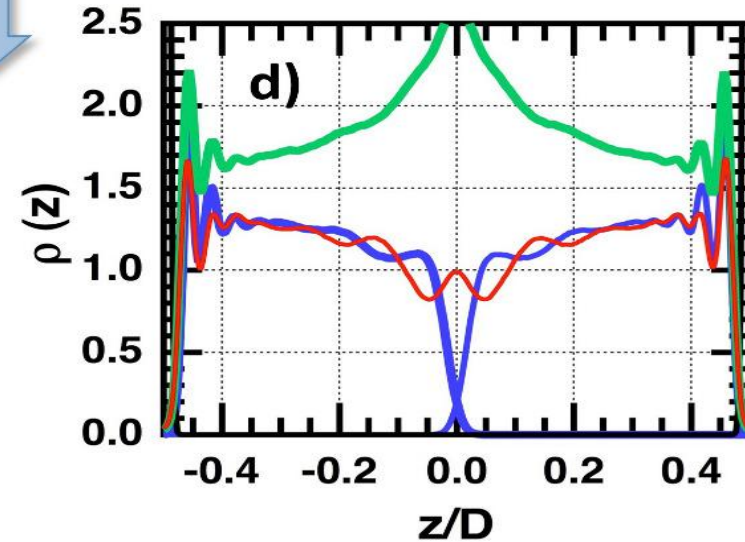
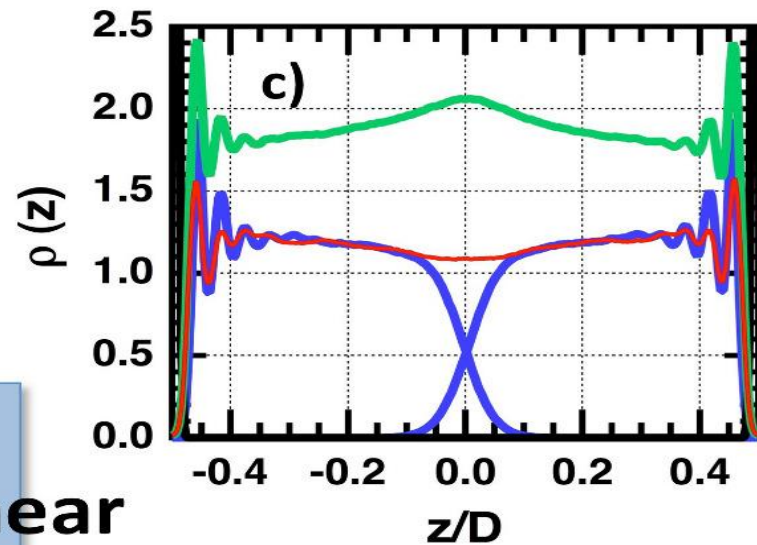
The effect of charge

Neutral brushes

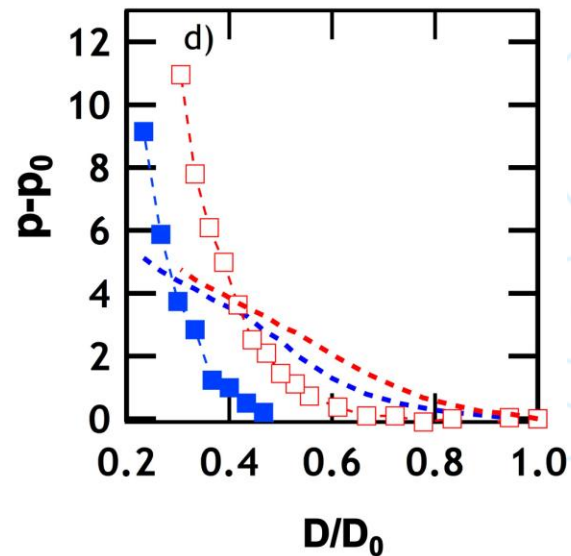
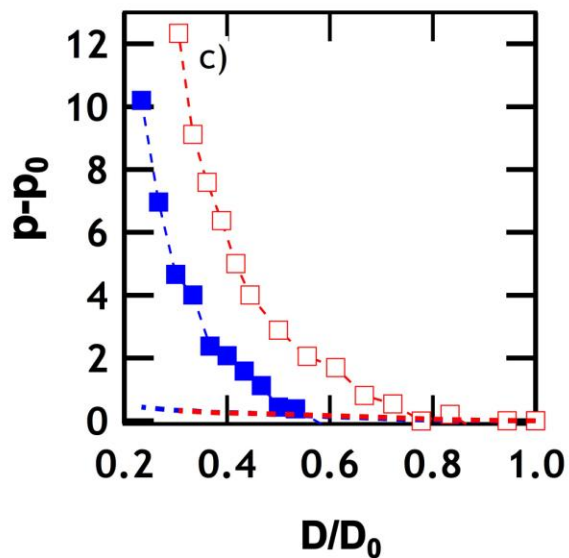
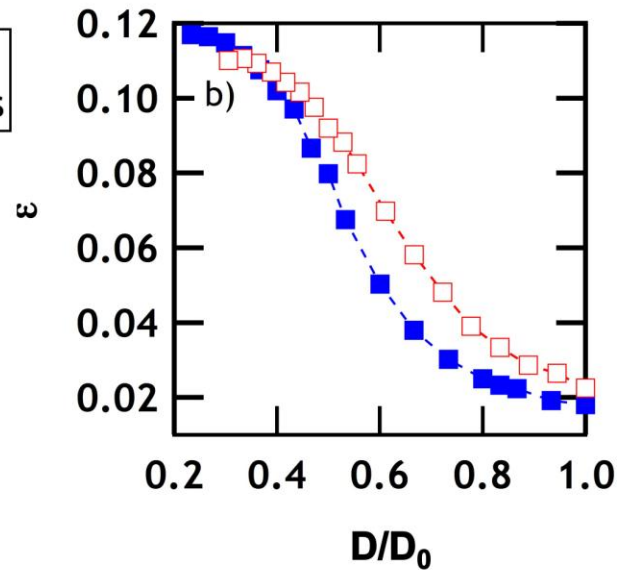
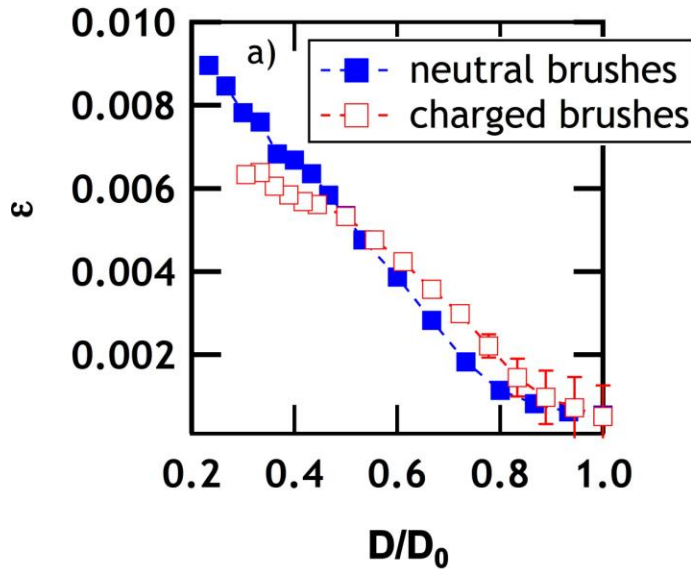


shear

Charged brushes



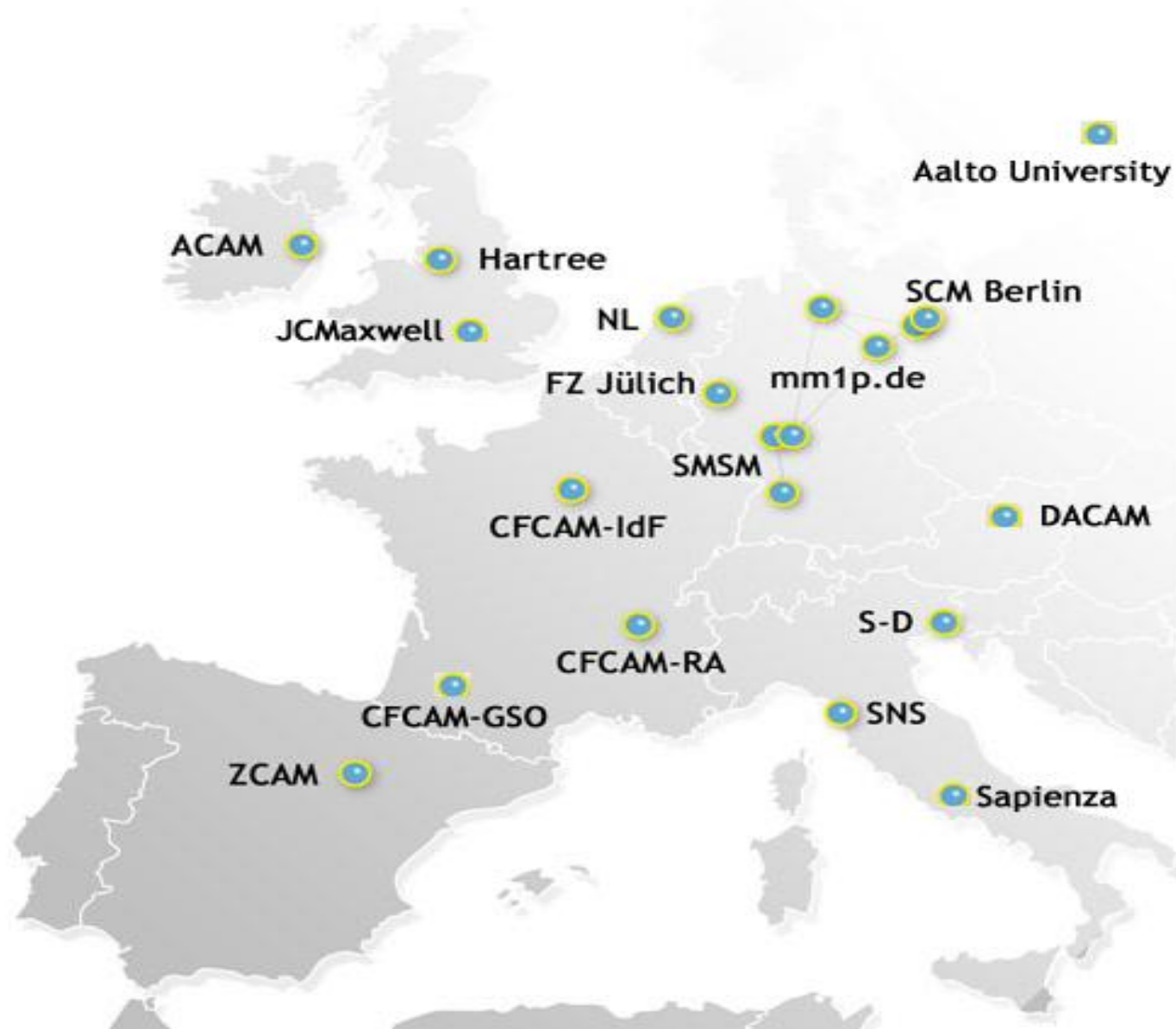
Charged and neutral brushes



The Node structure of CECAM



Greater Europe



The new Board of Directors

1. Gerhard Kahl	CECAM-AT	Austria
2. Mikko Alava	CECSM-FI	Finland
3. Ralf Everaers	CECAM-FR-RA	France
4. Fernand Spiegelman	CECAM-FR-GSO	France
5. Gilles Zérah	CECAM-FR-IdF	France
6. Burkhard Dünweg	CECAM-DE-SMSM	Germany
7. Luigi Delle Site	CECAM-DE-SCM	Germany
8. Thomas Frauenheim	CECAM-DE-MM1P	Germany
9. Godehard Sutmann	CECAM-DE-JUELICH	Germany
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11. Oded Hod	CECAM-ISR	Israel
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13. Carlo Casciola	CECAM-IT-SAPIENZA	Italy
14. Fredrico Becca	CECAM-IT-CARSO	Italy
15. Luuk Visscher	CECAM-NL	Netherlands
16. Michel Mareschal	CECAM-ES	Spain
17. Dominic Tildesley	CECAM-HQ	Switzerland
18. Mike Payne	CECAM-UK-JCMAXWELL	UK
19. Nick Harrison	CECAM-UK-HARTREE	UK

The work of the Board of Directors

- Creation of the annual programme
 - Finding Workshops, Tutorials, Sponsorship, and The CECAM Conference
 - Cross-referencing of the proposed programme
 - Ensuring the quality of the proposed programme
- Creation of a strong visitors programme
 - Encouraging visitors that will strengthen the existing research interests
 - Deliberately extending the CECAM zone of comfort
 - Joint research and grant applications between the nodes

New Areas for CECAM 2014

- computational biology (e.g. systems biology, cellular modelling, medicinal chemistry);
- simulations of the formation of defects in materials, the dynamics of dislocations and the propagation of cracks;
- the simulation and modelling of systems far from equilibrium;
- quantum dynamics
- multi-scale modelling of friction and wear between surfaces.

Some Conclusions



CECAM is

A superb location and facilities suitable for the leading European think-tank in atomic and molecular modelling

A 45 year heritage in providing thought-leadership and training in its fields of interest

A network of nodes that give CECAM influence right across Europe

Strong support from the EPFL and Switzerland in hosting the CECAM Headquarters

A dedicated and efficient staff

A rich, well-balanced and diverse programme of activities

A stable plan for growth

CECAM could be

- A faster and slicker machine for getting hot topics in simulation discussed widely and in a timely fashion
- The trusted partner of the EU in discussions on materials and biological modelling for the Horizon 2020 programme
- A catalyst for industry to be more closely in the development of workshops and tutorials by considering
 - the training needs of industrialists
 - the long term research needs of industry in our space;
 - industrial sponsorship of node and centre activities.

Mission

- CECAM is 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.
- Over the last twenty years, powerful advances in computer hardware and software have supported the extension of these methods to a wide range of problems in materials science, biology and medicinal chemistry.
- The current call for 2014 proposals ends on 14 July 2013. Log on to the CECAM website (www.cecarn.org) and submit a proposal. It could not be easier.
- Thanks for your attention!!