Soft matter computational modeling

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ARTICLE PREVIEW

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Soft-matter miracles

David Quéré

Nature **465**, 1011 (24 June 2010) | doi:10.1038/4651011a
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Matière sensible: Mousses, gels, cristaux liquides et autres miracles (Sensitive Matter: Foams, Gels, Liquid Crystals and Other Miracles)
by Michel Mitov
Seuil: 2010. 179 pp. €18

Soft-matter research investigates ambiguous states of matter, the paradoxical properties of which rely on the art of mixture. An emulsion formed simply of oil and water plus a few molecules of detergent gains the stability of a cream. Similarly, foam produced from air bubbles in soapy water transforms those two fluids into an almost-solid state. In *Matière sensible*, liquid-crystal researcher Michel Mitov marvels at the surprising behaviour of these materials.

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Rather than naming the book after his discipline, Mitov uses the title 'sensitive matter'. The expression 'soft matter' was coined as a joke in the 1970s by physicist Madeleine Veyssié — indeed, the French term *matière molle* sounds sleazy. However, it acquired a majesty when physicist Pierre-Gilles de Gennes chose it as the title of his Nobel lecture in 1991. From then on, the scientific community was converted.

Introduction

- Focus
  - Projects
  - Persons
- OMM (VR Linnaeus research environment)
- Simulation method
  - Molecular dynamics
  - Monte Carlo simulation
  - Stochastic dynamics
- Theory
  - Liquid-state theory
  - Various mean-field theories

Soft matter computational modeling

PAST MAIN RESEARCH INTEREST

	Topic	Group members
1	Charged colloids	V. Lobaskin, J. Rescic
2	Polymer at interfaces	M. Skepö, N. källrot, M Patra
3	Colloid-polymer systems	M. Skepö, A. Akinshina
4	Oppositely charged polyions	Y. Hayashi
5	Charged diblock copolymers	A. Akinshina, N. Shusharina
6	Polyelectrolyte gels	S. Schneider, S. Edgecombe
7	Protein modeling	F. Carlsson, M. Jönsson
8	Virus and confinement	D. Angelescu

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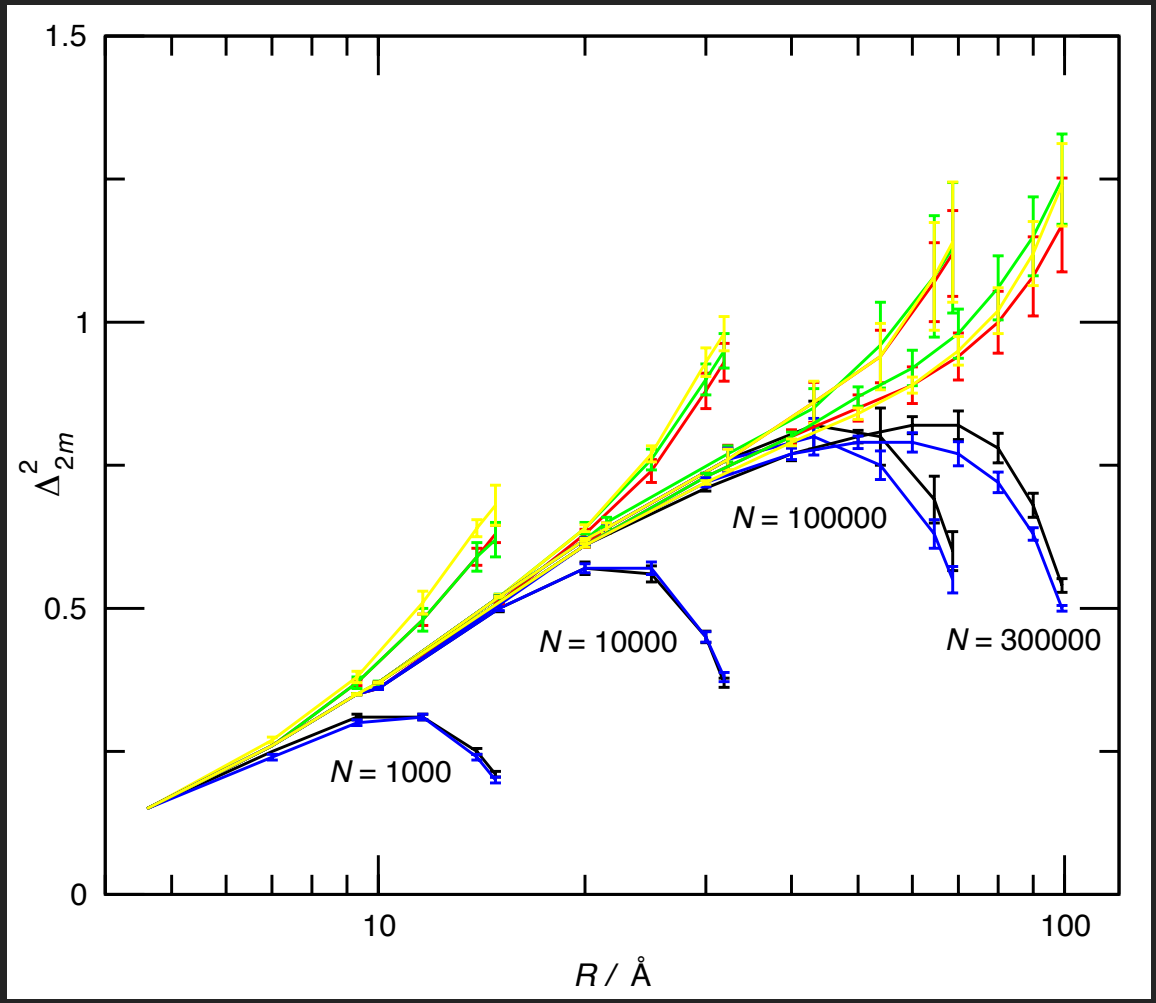
CURRENT MAIN RESEARCH INTEREST

	Topic	Group member	
1	Dipolar fluids and b.c.	Joakim Stehammar	PhD
2	Virus self-assembly	Ran Zhang	Post-doc
3	Solutions of dipolar particles	Alexei Abrikossov	Proj. ass.
4	Hierarchical polymers	Erik Wernersson	Post-doc
5	Dendrimer adsorption	Marianna Yanez	PhD
6	Development and distribution of statistical-mechanical software		

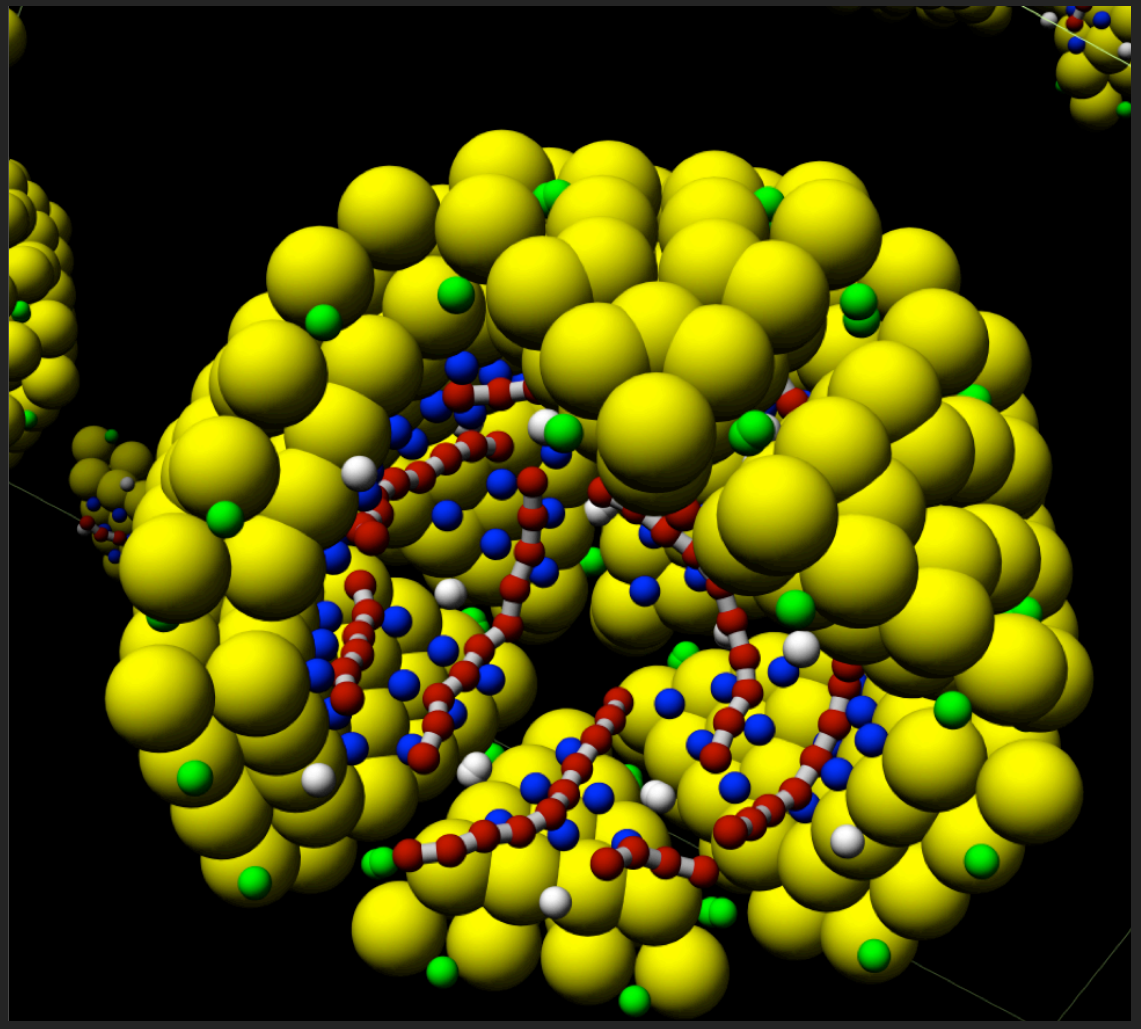
Dipolar fluids and boundary conditions



Joakim Stenhammar, Gunnar Karlström, and Per Linse

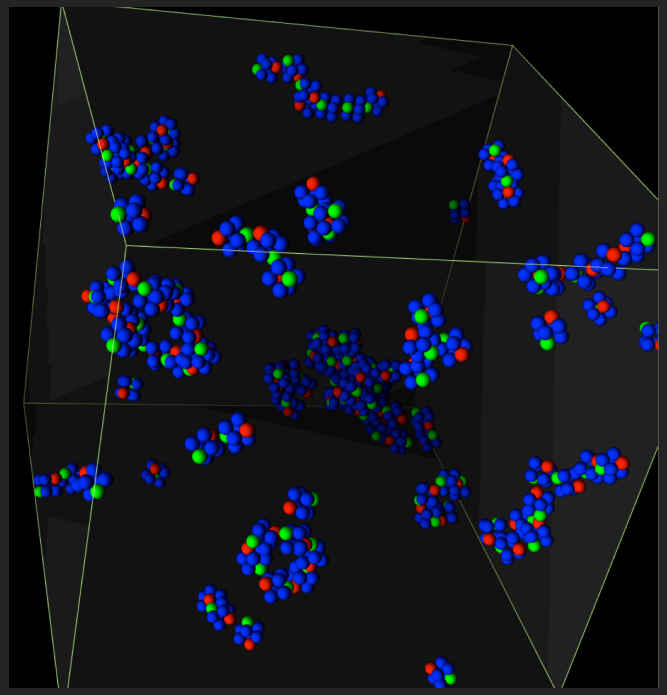
JPCM 2008, JCP 2009, JCP 2009, JCP 2010, JPCB 2010,
Mol. Phys. 2011, CPL 2011, JCP 2011, JCTC 2011

Virus self-assembly

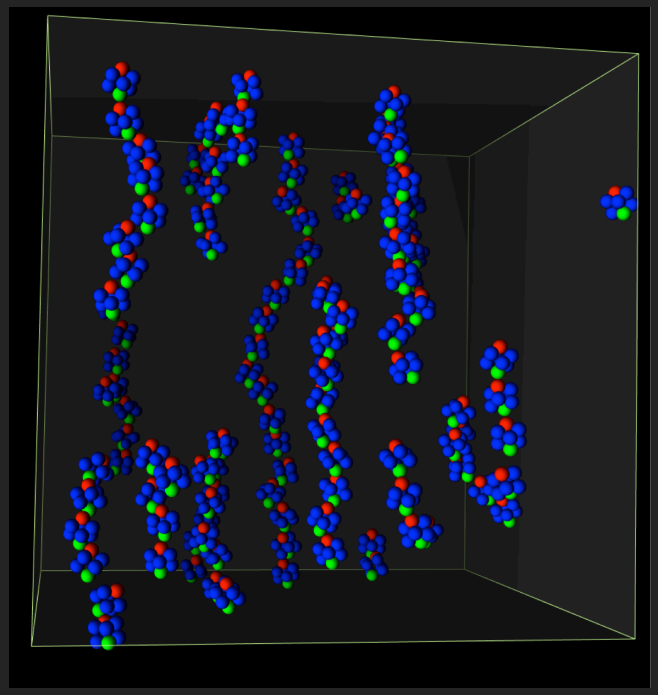


Ran Zhang

Solutions of dipolar particles



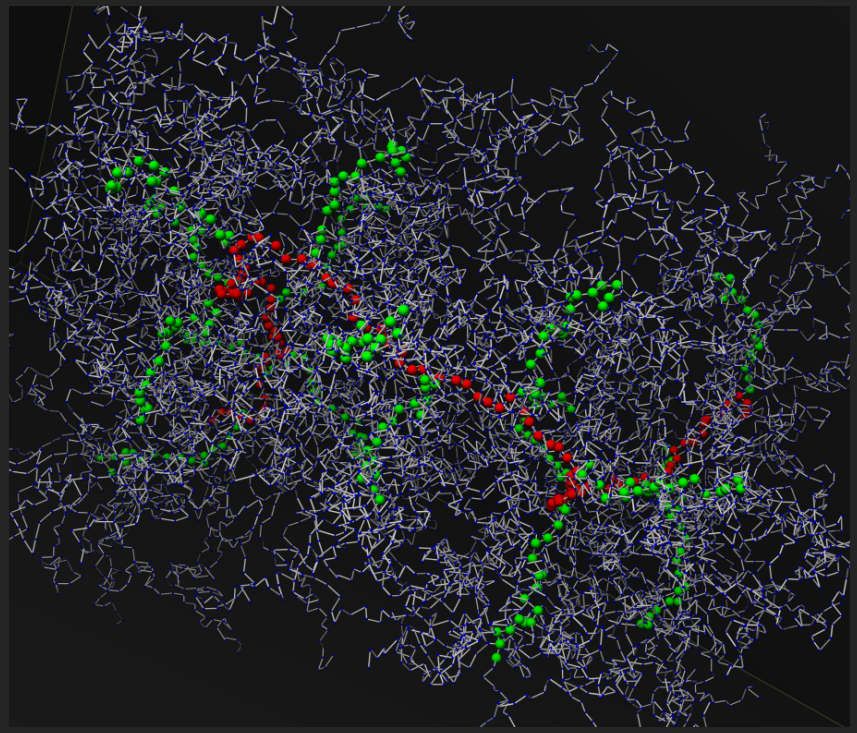
no field



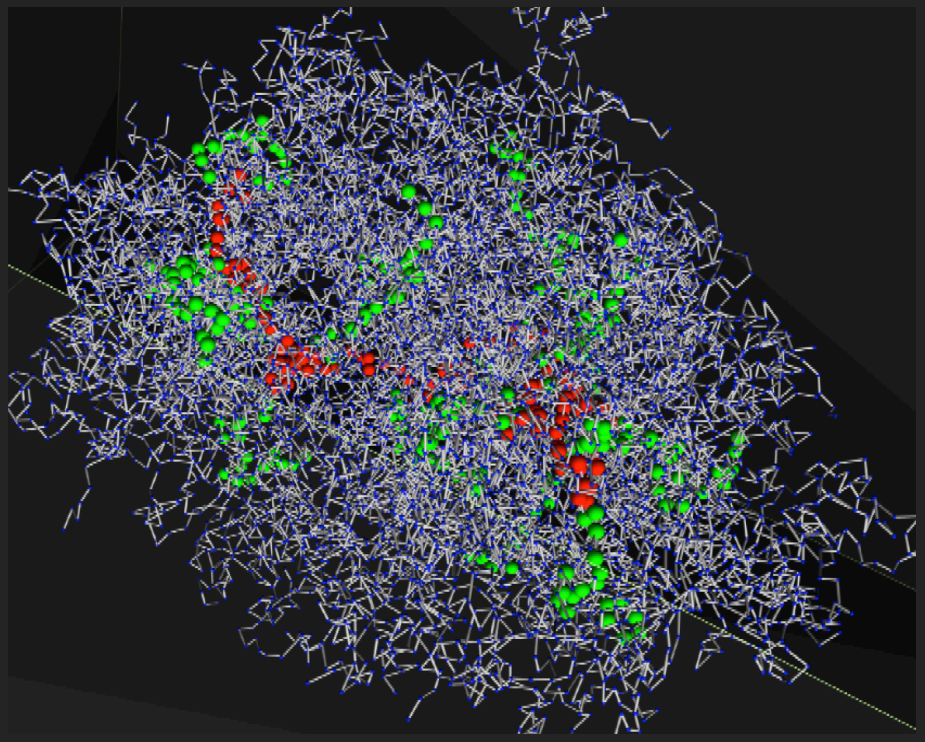
with field

Alexei Abrikossov
(in collaboration with Albert Philipse et al.)

Hierarchical polymers



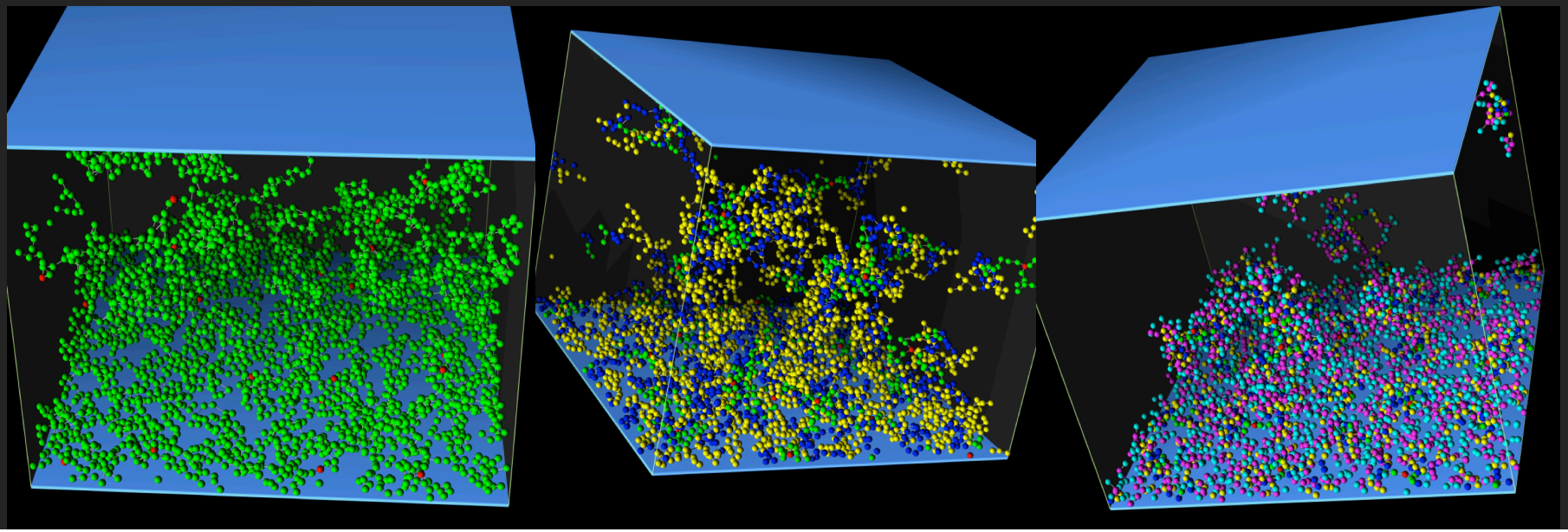
good solution

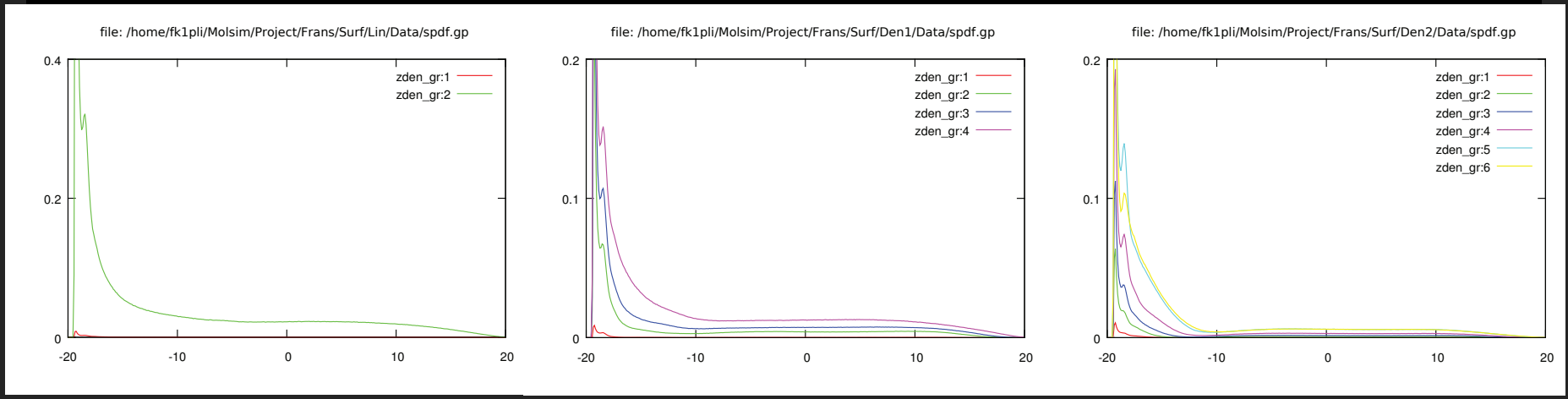


poor solution

Erik Wernersson
(in collaboration with Per Claesson et al.)

Dendrimer adsorption





Marianna Yanez, Per Linse and Frans Leermakers

Software

(web portal: www.fkem1.lu.se/sm)

- DIELEC
  - a software for calculation of the electrostatics in the presence of spherical dielectric discontinuities.
- MOLSIM
  - a software for **molecular dynamic**, **Monte Carlo**, and **Brownian dynamic** simulation and for analyzing simulation data of molecular systems for an extended set of conditions
- OZ
  - a software for numerically solving the **Ornstein-Zernike** equation with a closure for homogeneous systems with particles possessing central forces
- PB
  - a software for numerically solving the one-dimensional **Poisson-Boltzmann** equation for infinite and finite systems of different symmetries
- PGSE
  - a software for simulation of **pulse-gradient spin-echo** attenuations for spins diffusing in restricted spaces of different symmetries with permeable walls
- POLYMER
  - a software for solving **lattice mean-field models** containing a mixture of solvents and polymers for homogeneous (Flory-Huggins theory) and heterogeneous (Scheutjens-Fleer theory) solutions extended to polymers possessing internal degrees of freedom

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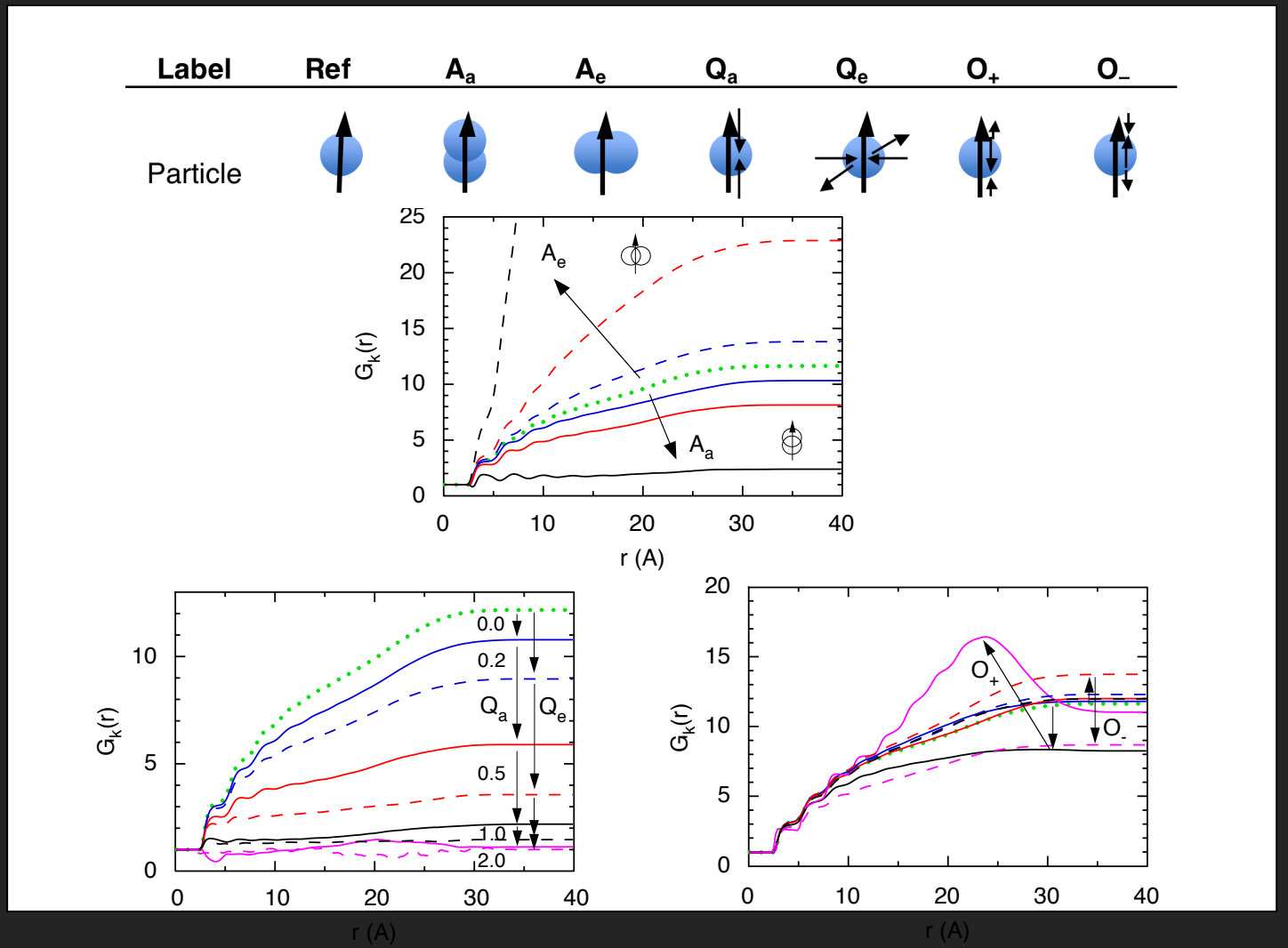
OTHER RESEARCH INTERESTS

	Topic	Principal collaborator
1	Dipolar fluids	Gunnar Karlström
2	Dielectric boundary cond.	Leo Lue
3	Folding of helical peptides	Thomas Bleha
4	Particle adsorption	Håkan Wennerström
5	Magnetic particles	Albert Philipse
6	Bottle-brush adsorption	Per Claesson
7	Polyelectrolyte complex.	Rita Dias

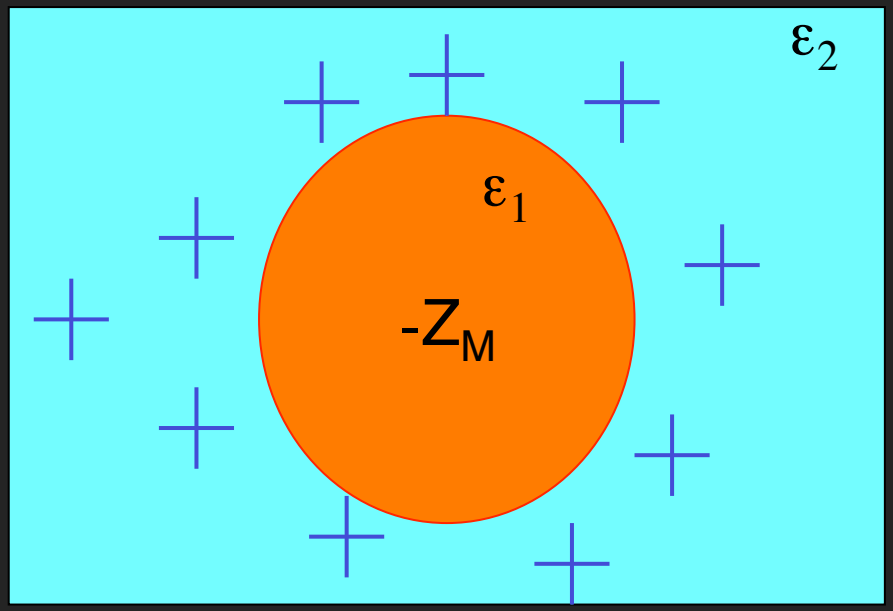
Dipolar fluids

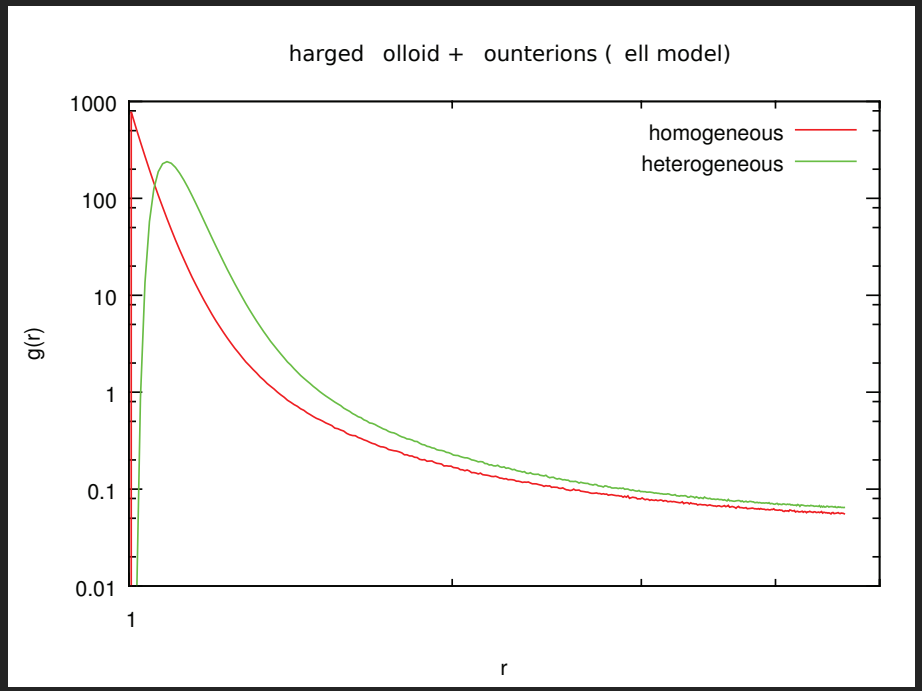


Gunnar Karlström and Per Linse

JCP 2010, JCP 2010, J Stat Phys 2011, J Stat Phys 2011

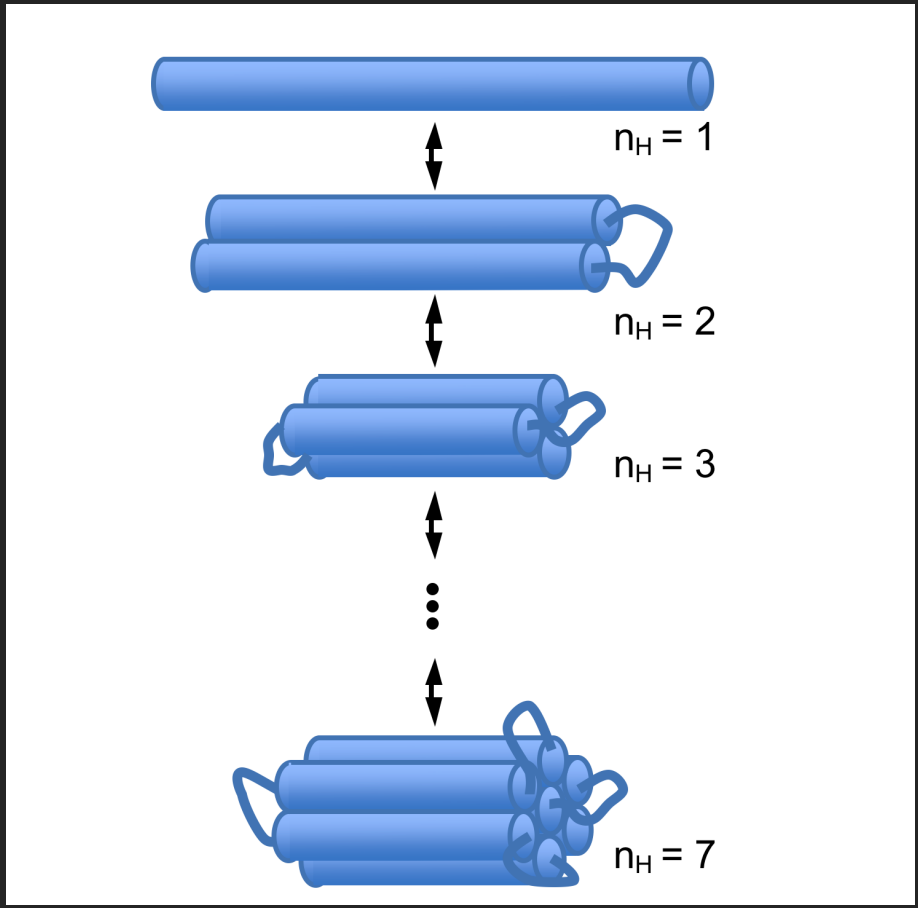
Dielectric boundary conditions





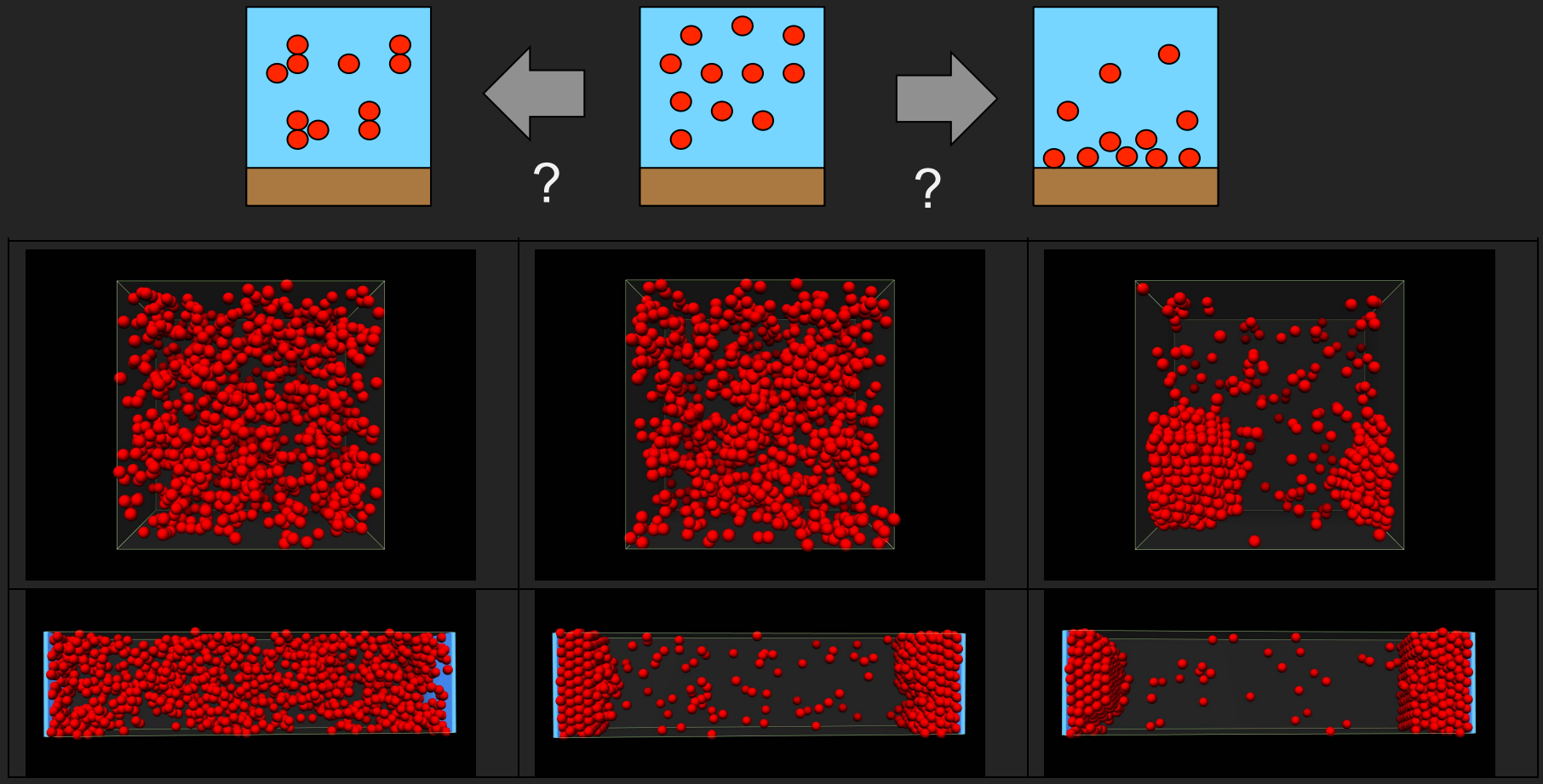
Leo Lue and Per Linse
JCP 2011

Folding of helical peptides



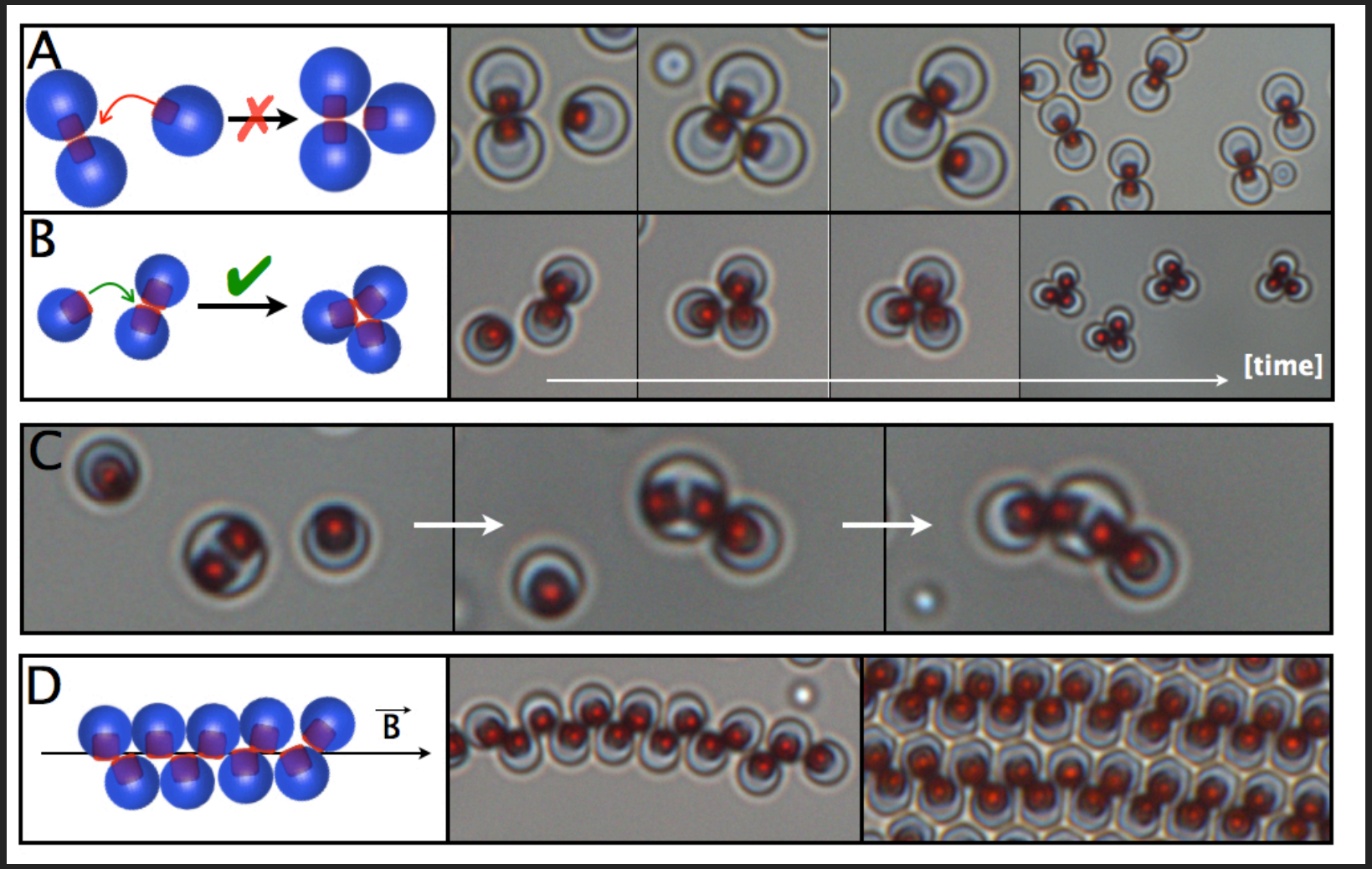
Per Linse, Peter Palencar, and Thomas Bleha
JCPB 2011

Particle adsorption on solid surfaces



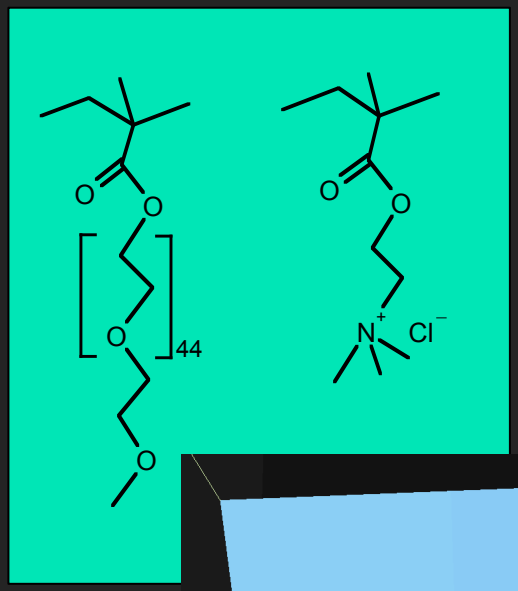
Per Linse and Håkan Wennerström
Soft Matter 2012

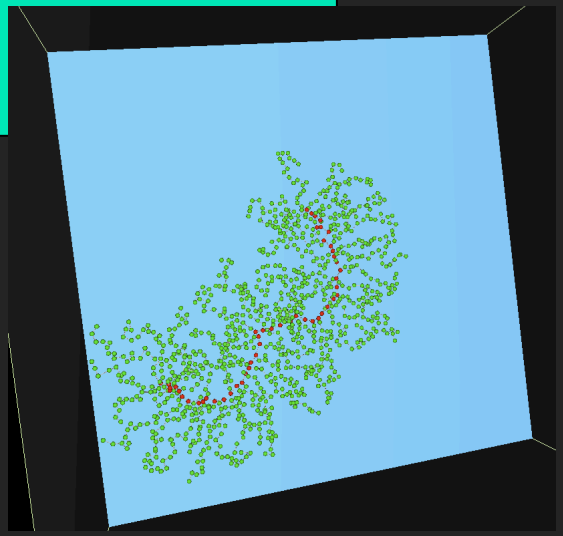
Solution of magnetic particles

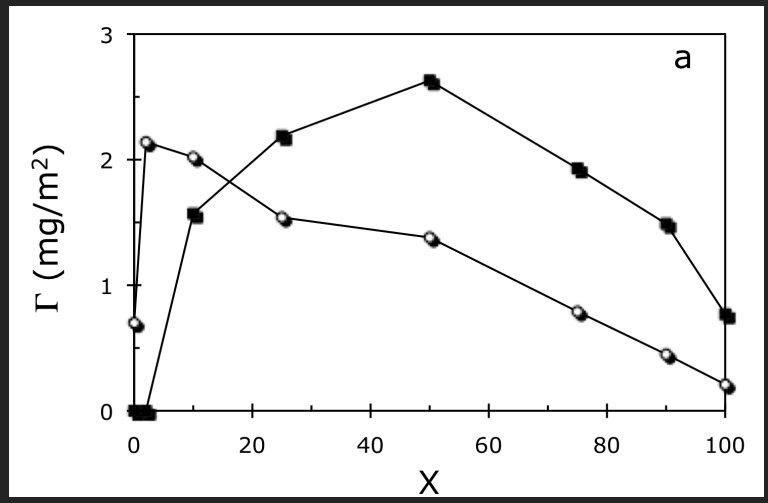


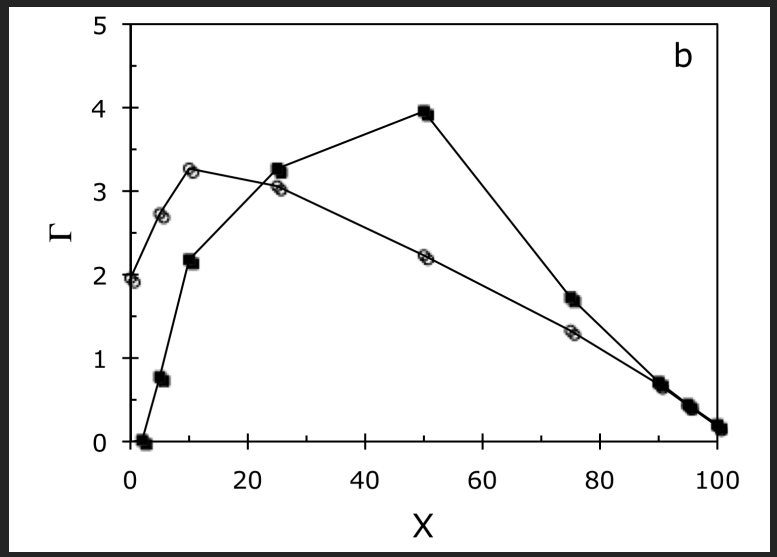
Experimental results: Stefano Sacanna et al.
Modeling: Alexei Abrikossov

Hierarchical polymers



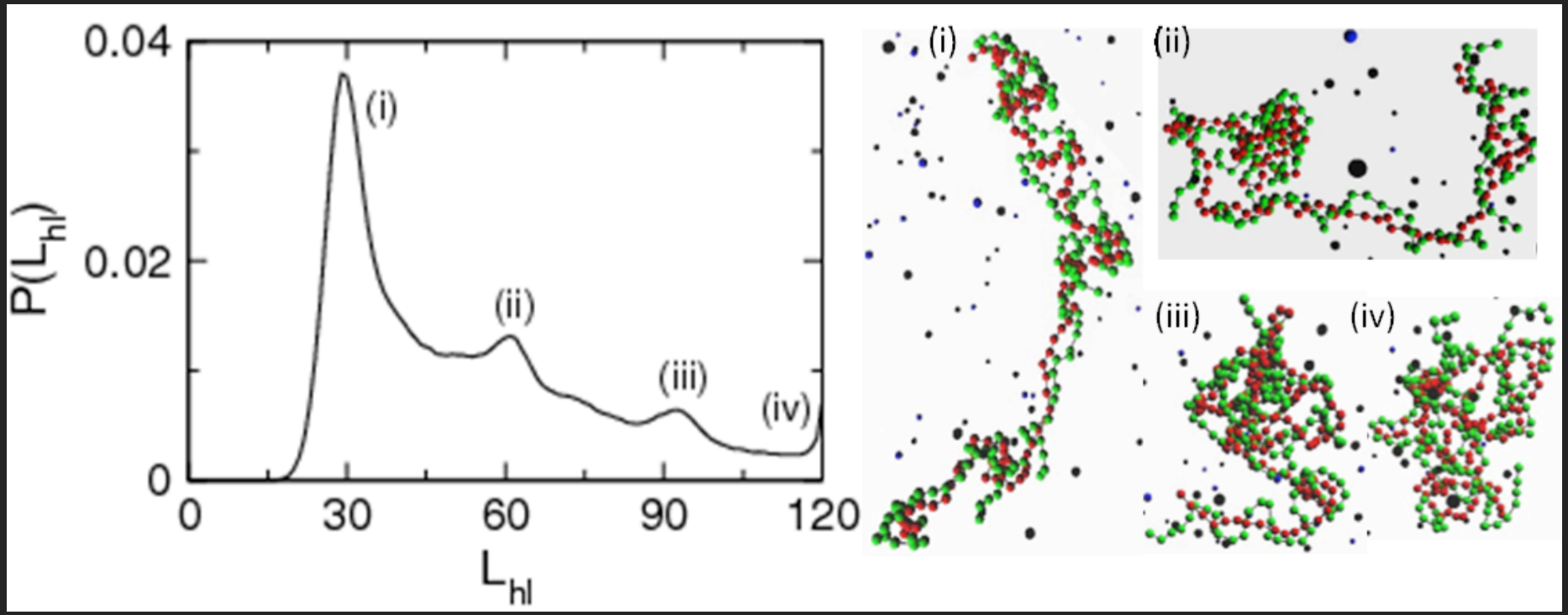






Per Claesson and Per Linse
MA 2009, MA 2010

Polyelectrolyte complexation



Rita Dias, Per Linse, and Alberto Pais
JCC 2011