An overview of the school on *Multiscale modeling and simulation in Hard and Soft Materials*

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- It is assumed that every one here is familiar with modeling at some length and time scale.
- Familiarity with basic concepts in statistical mechanics is assumed.
- Apart from the lectures there will be a separate interactive session with the speakers.

What do we mean by modeling at different length and time scale ?

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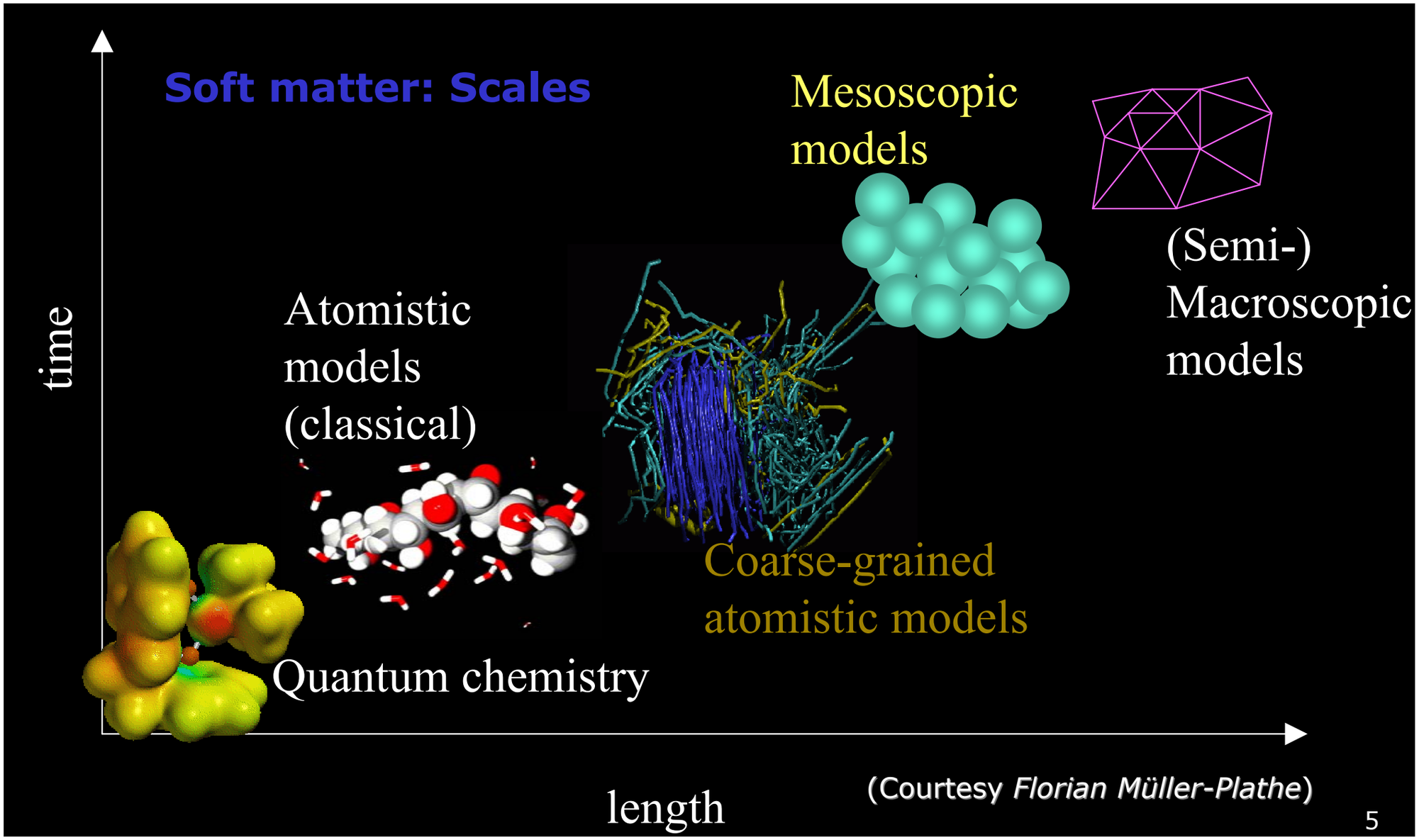

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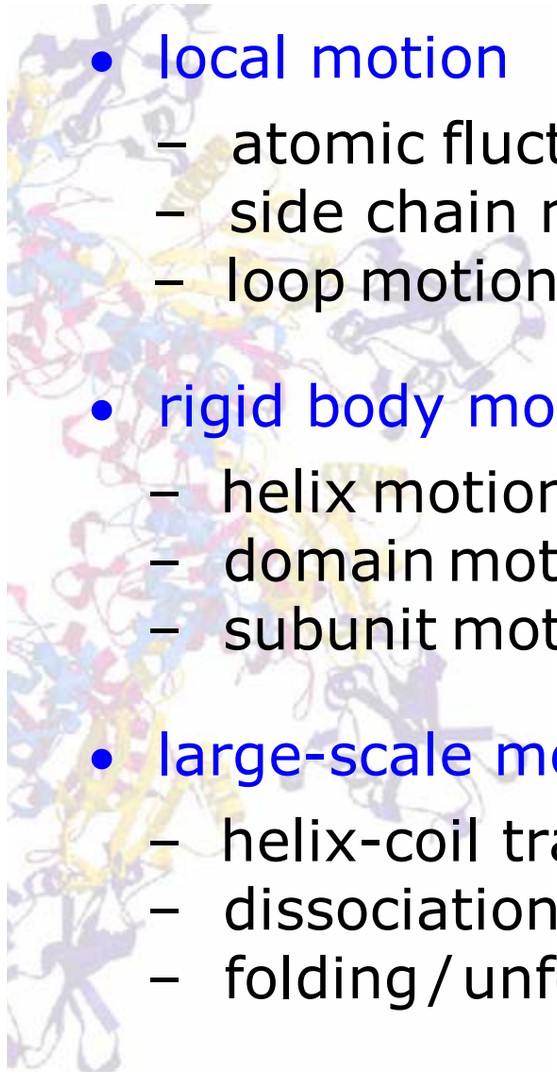

- local motion 10^{-3} ... 50 nm, 10^{-15} ... 10^{-1} s
  - atomic fluctuations
  - side chain motion
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  - helix motion
  - domain motion (hinge bending)
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- large-scale motion > 50 nm, 10^{-7} ... 10^{4} s
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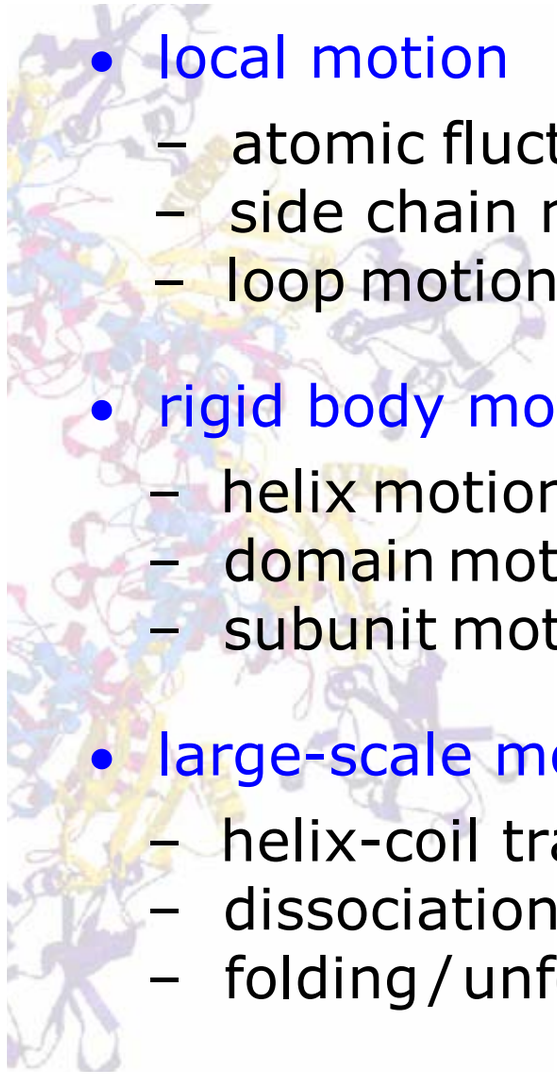
For example in protein dynamics, Peter Bolhuis



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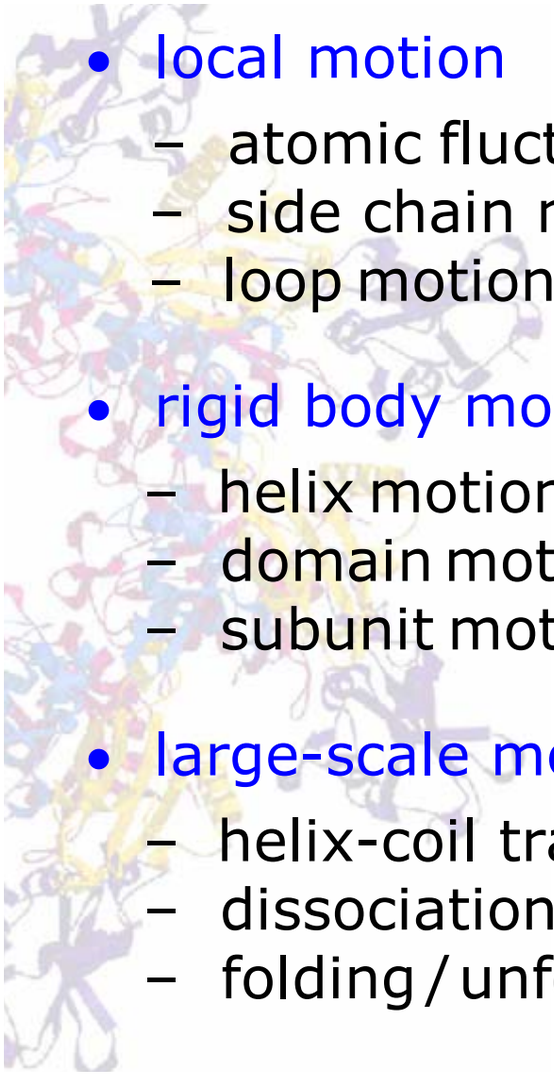

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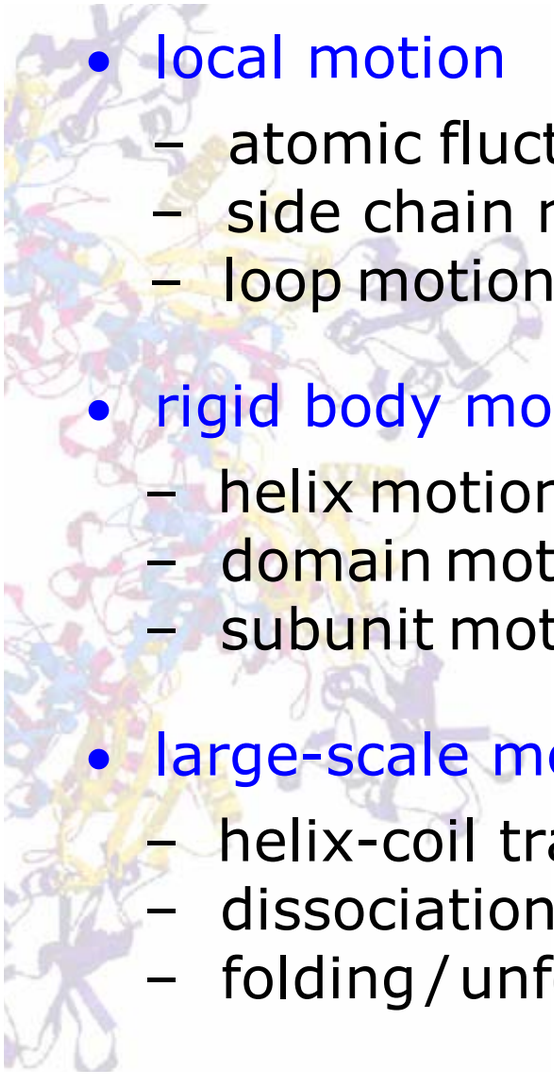

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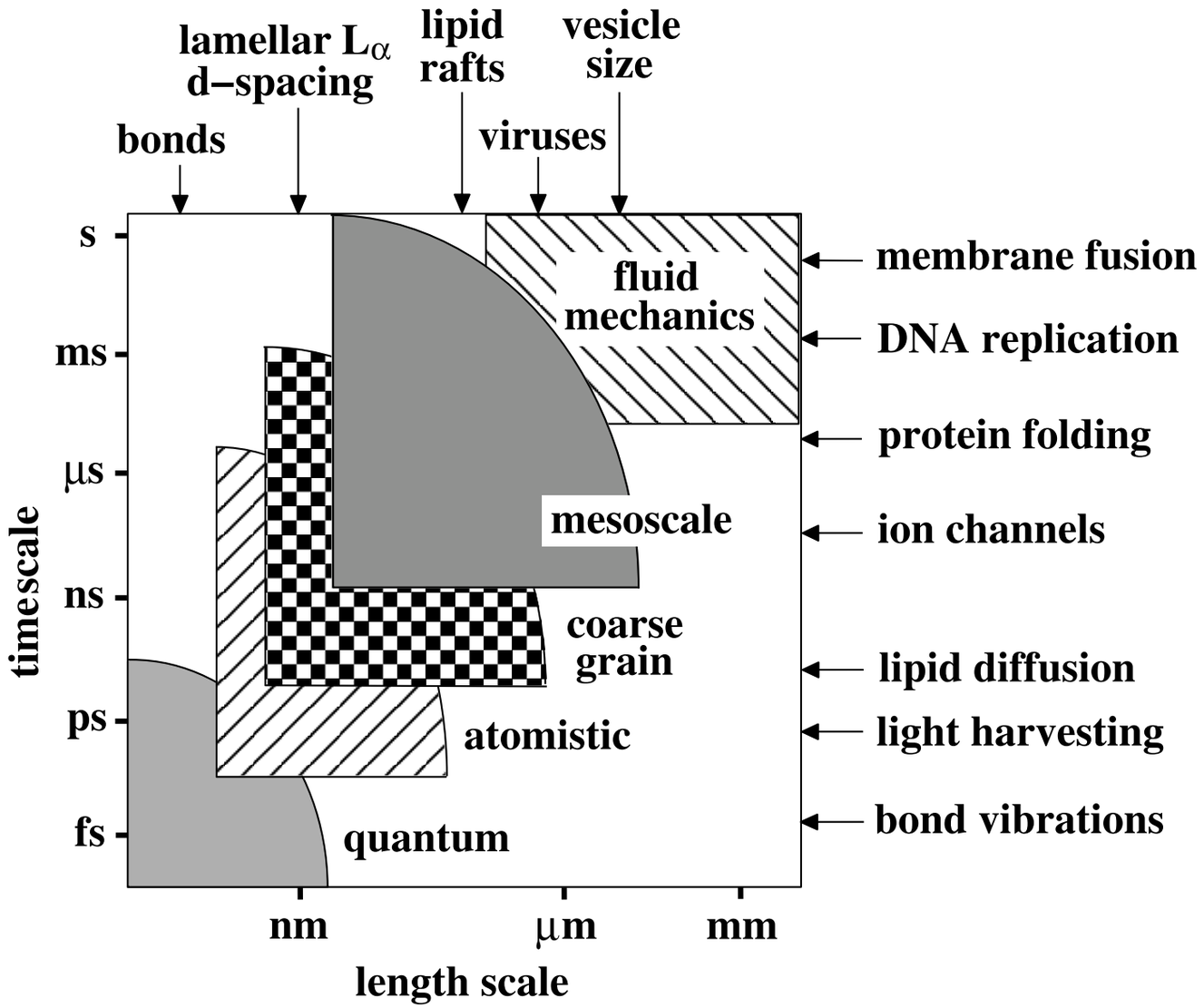

S.O. Nielsen, C.F. Lopez, G. Srinivas, and M.L. Klein, "Coarse grain models and the computer simulation of soft materials", *J. Phys.: Condens. Matter* **16** (2004) R481

What are Multiscale models

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“In engineering, physics, meteorology and computer science, multiscale modeling is the field of solving physical problems which have important features at multiple scales, particularly multiple spatial and(or) temporal scales. Important problems include scale linking” (Wikipedia)

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- Continuum models

Some challenges in soft matter

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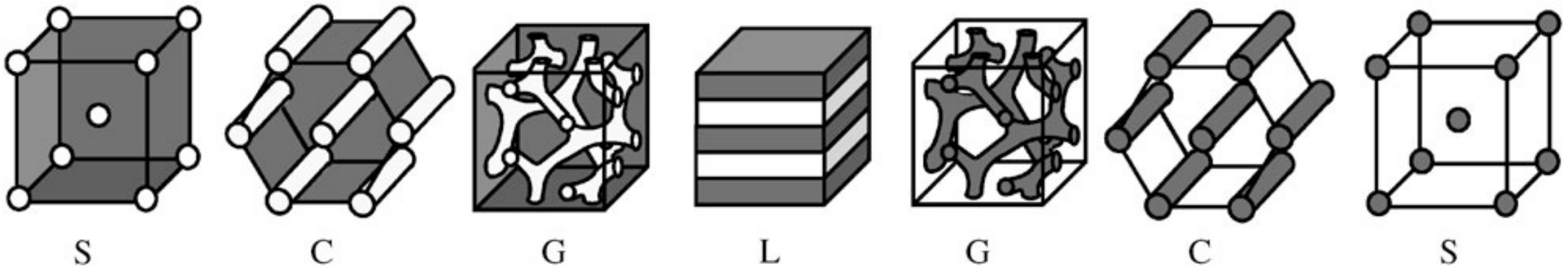

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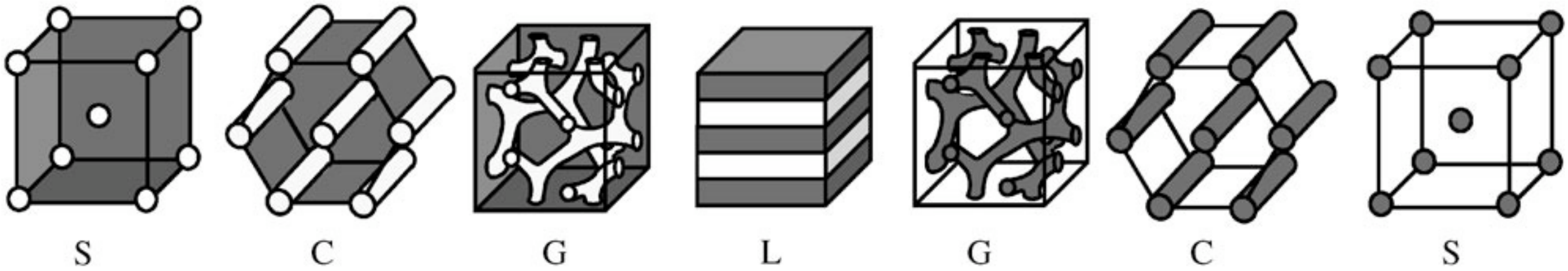

Schematic illustration of the nanostructures formed by an AB diblock copolymer in the bulk.
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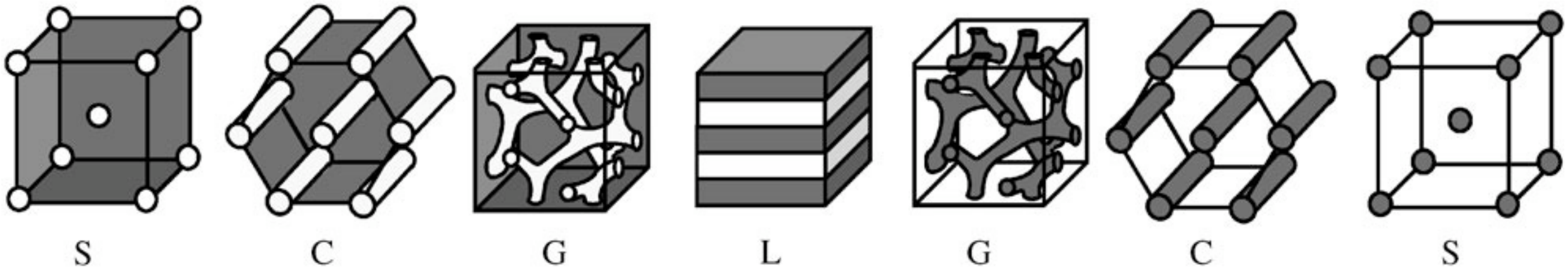

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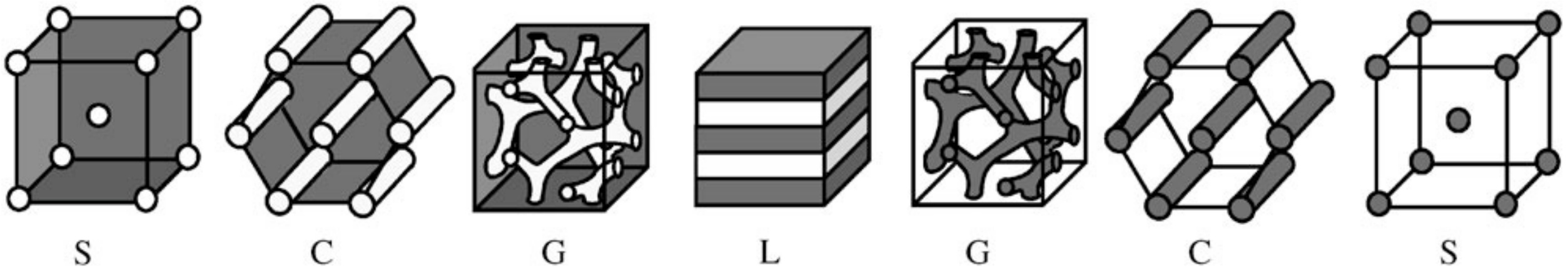

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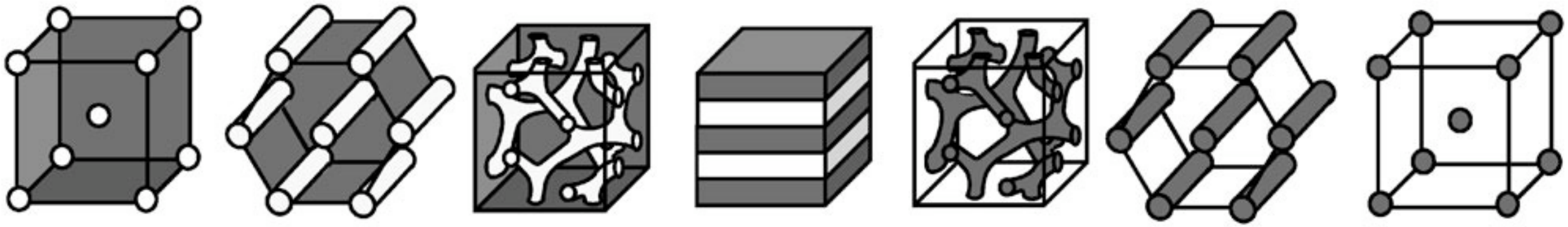

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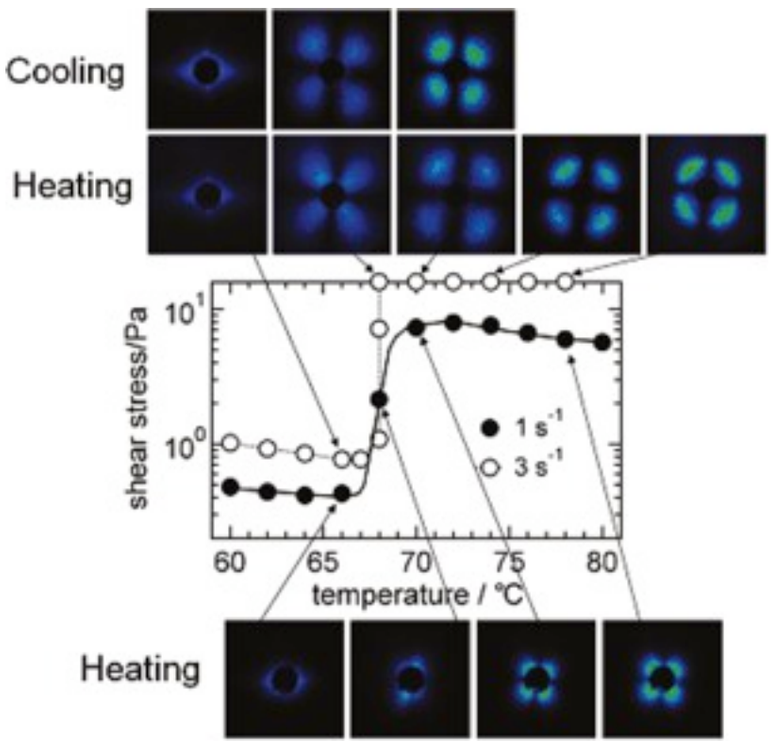

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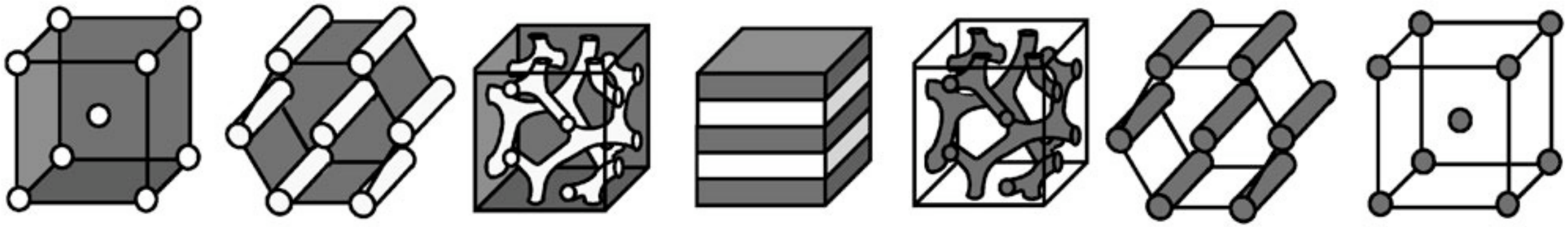

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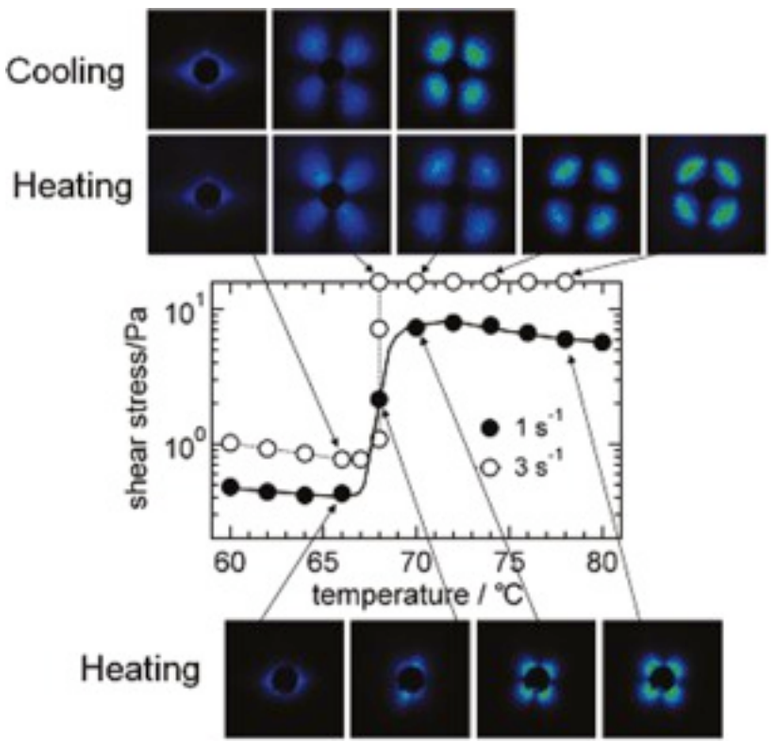

Lamellar to onion transition : Temperature dependences of the shear stress and 2-D depolarized SALS patterns at shear rates of 1 s-1 (b) and 3 s-1 (O) for the sample containing 48 wt%C16E7 in D2O.

Yuriko Kosaka et al Langumuir DOI: 10.1021/la903251v

Challenges in soft matter .....

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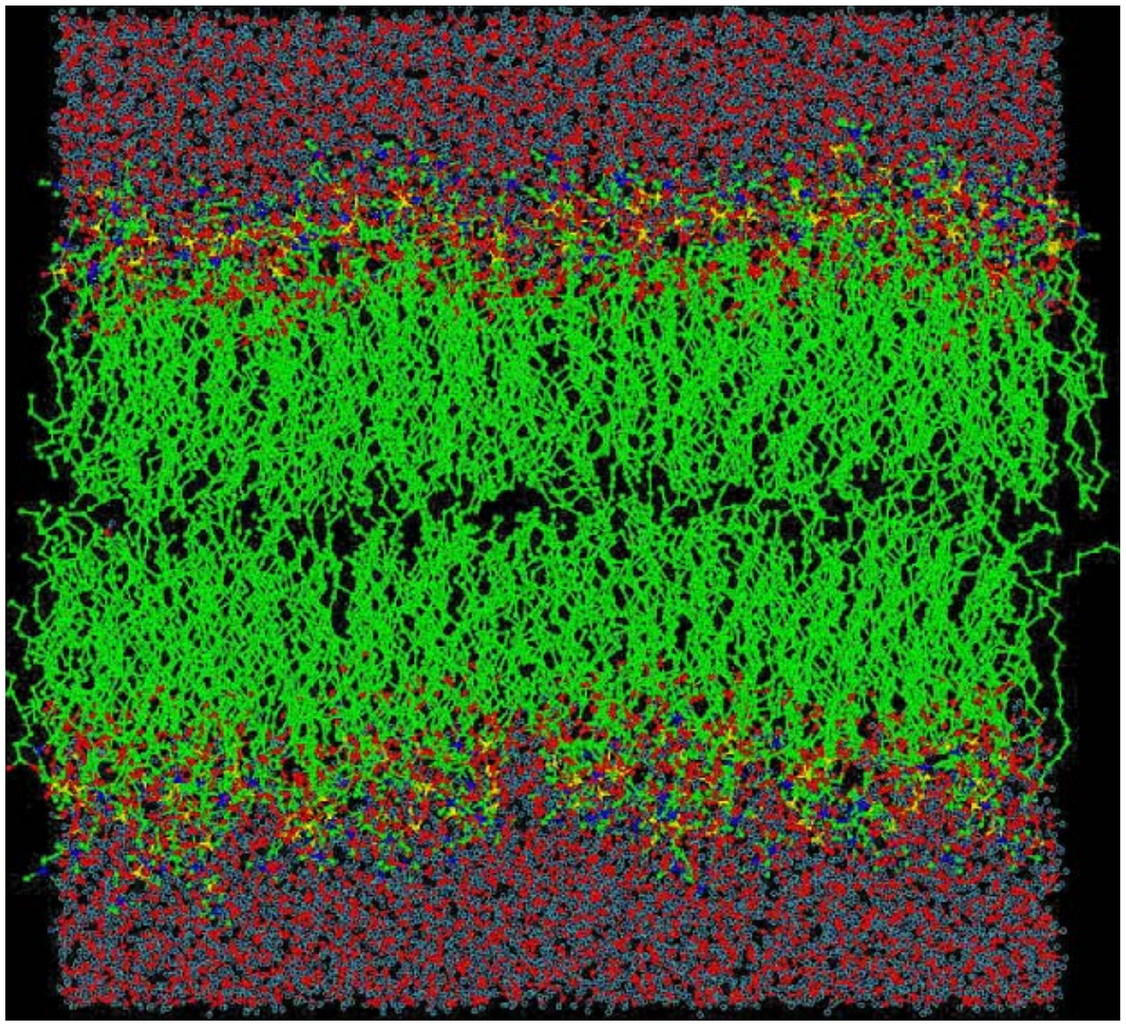

MD simulations of DPPC bilayer: 256 DPPC molecules , 6888 water molecules, Box size 90X80X75 $Å^3$ NPT ensembles, GROMOS force field, rigid bonds by SHAKE, electrostatics by Ewald

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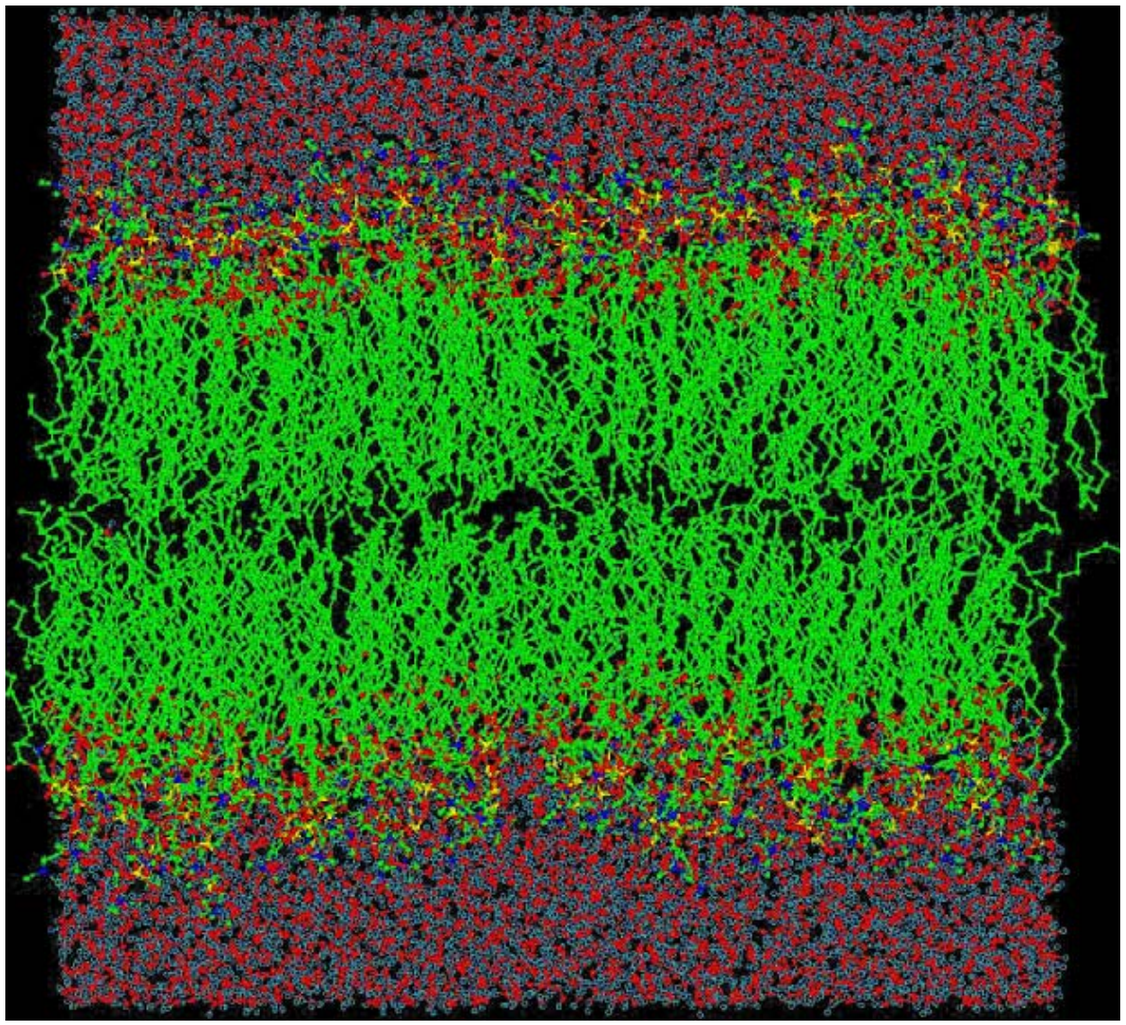

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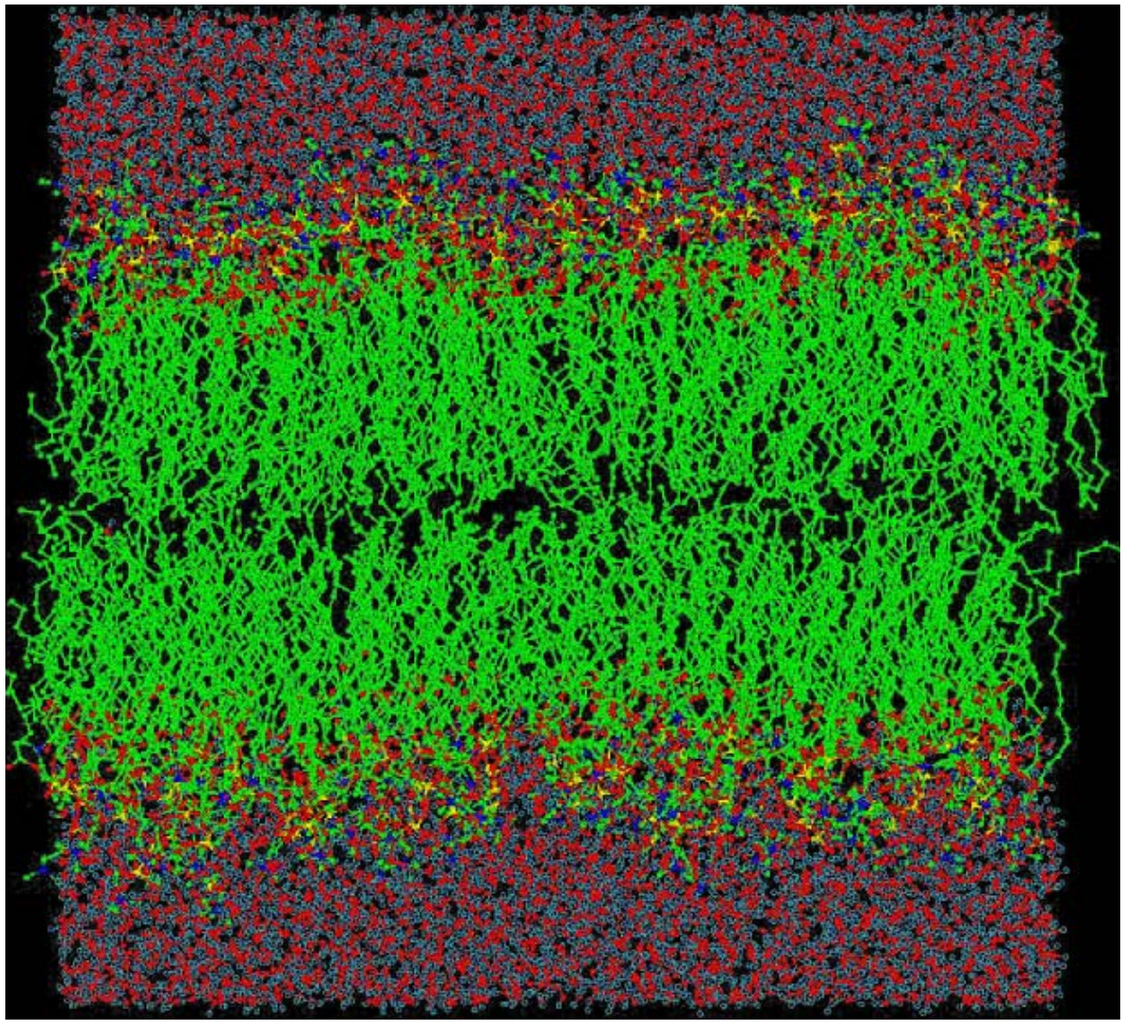

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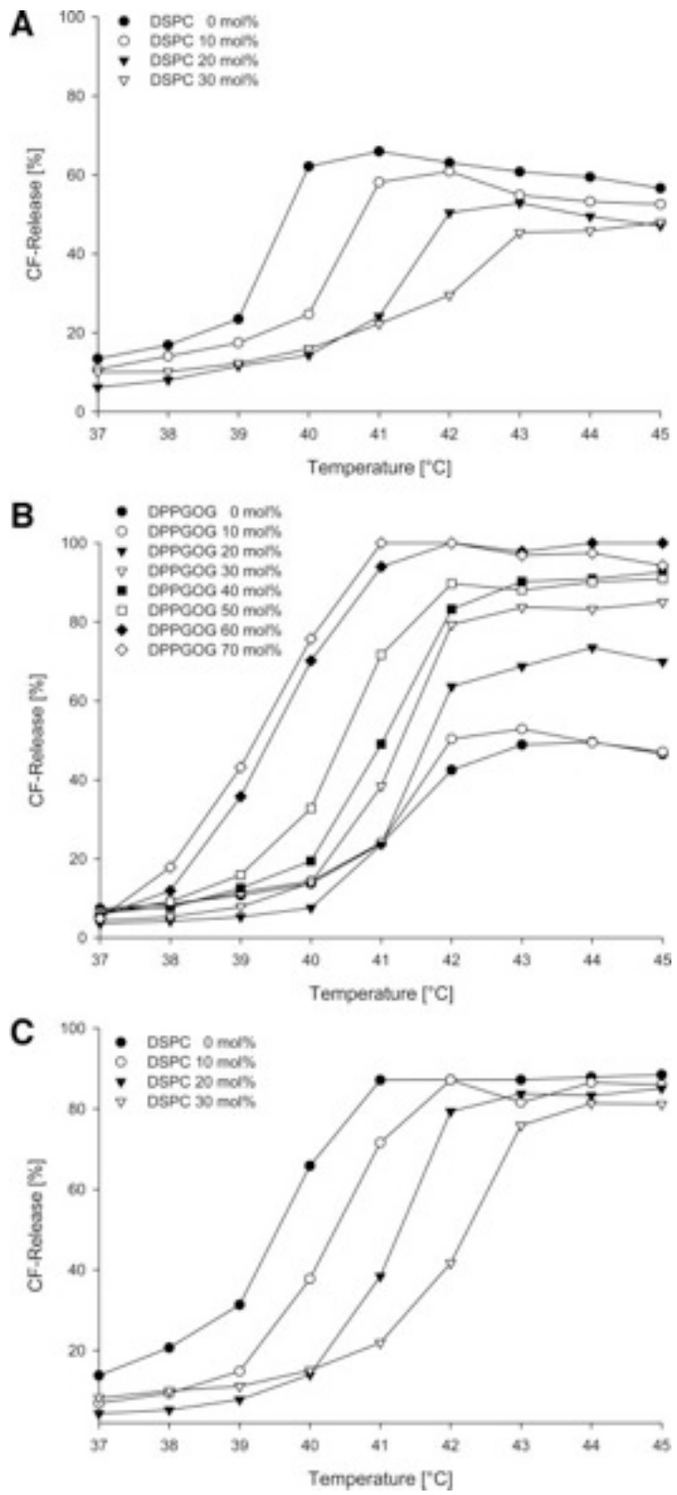
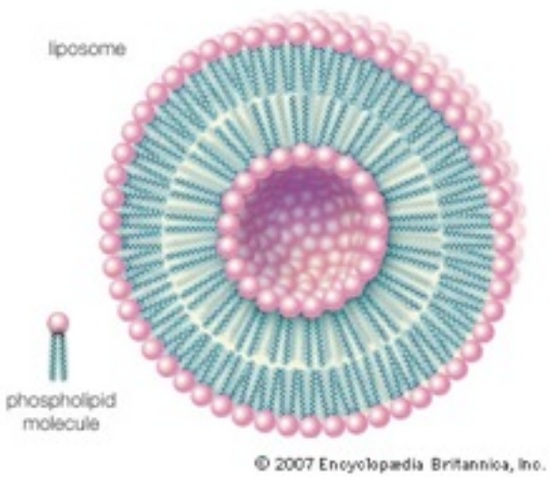


Temperature Sensitivity of Liposomes

L.H. Lindner Clinical Cancer Research **10**,2168 (2004)



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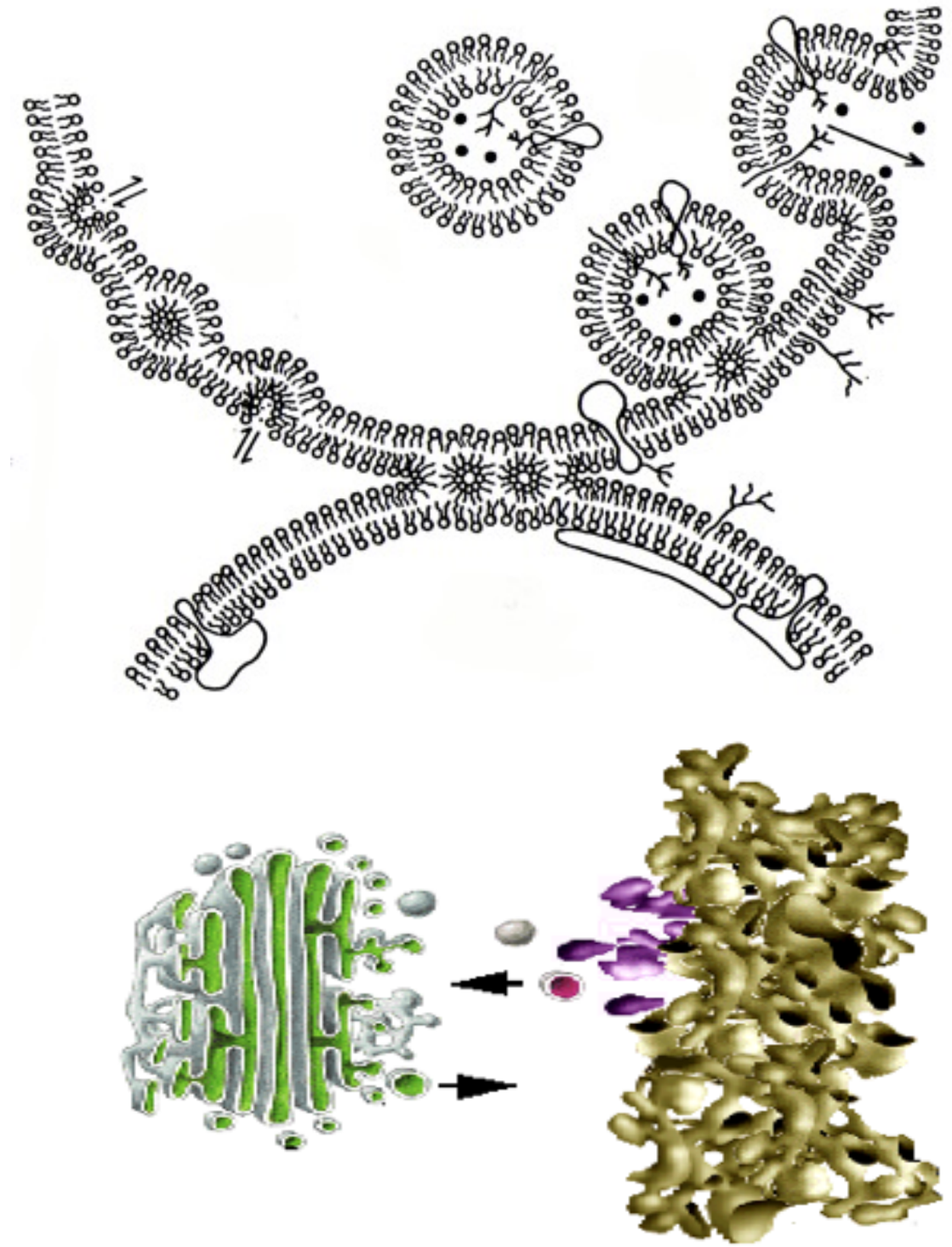

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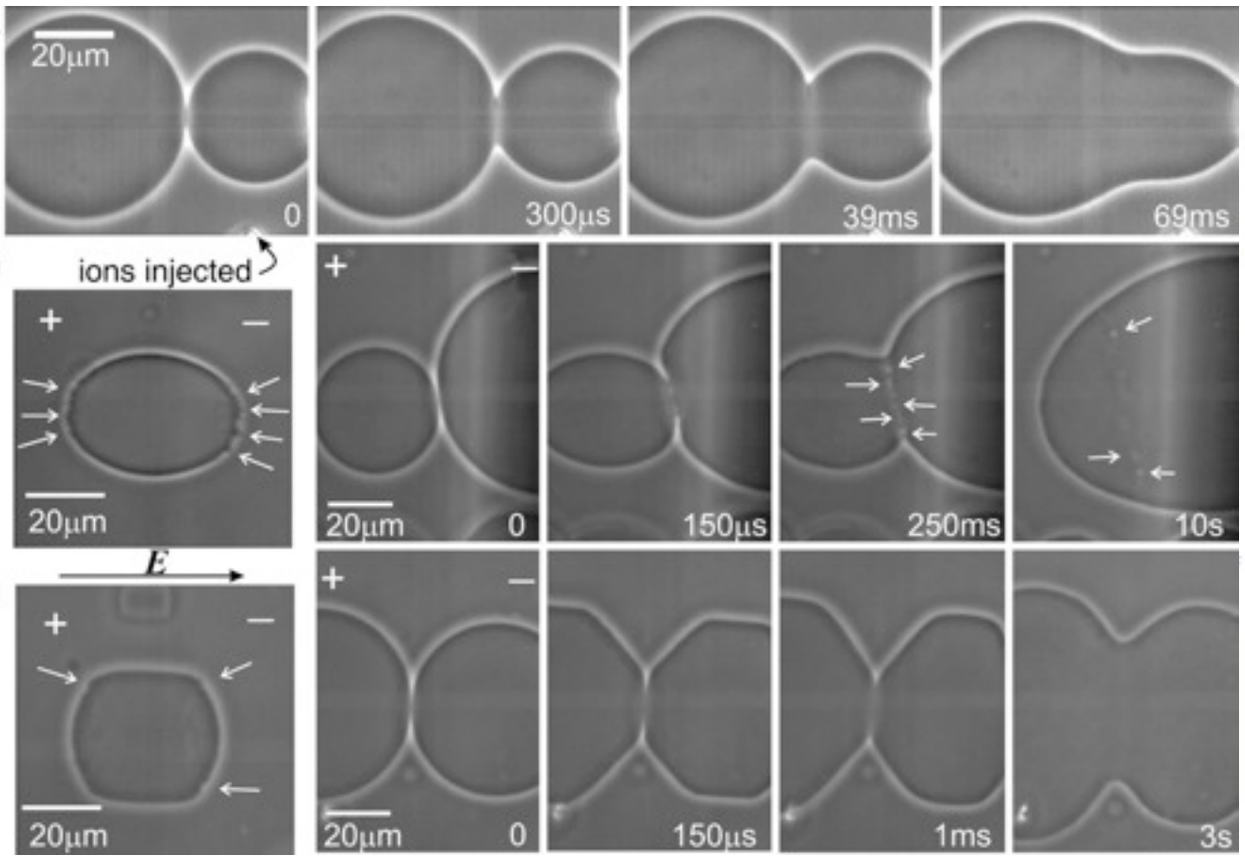
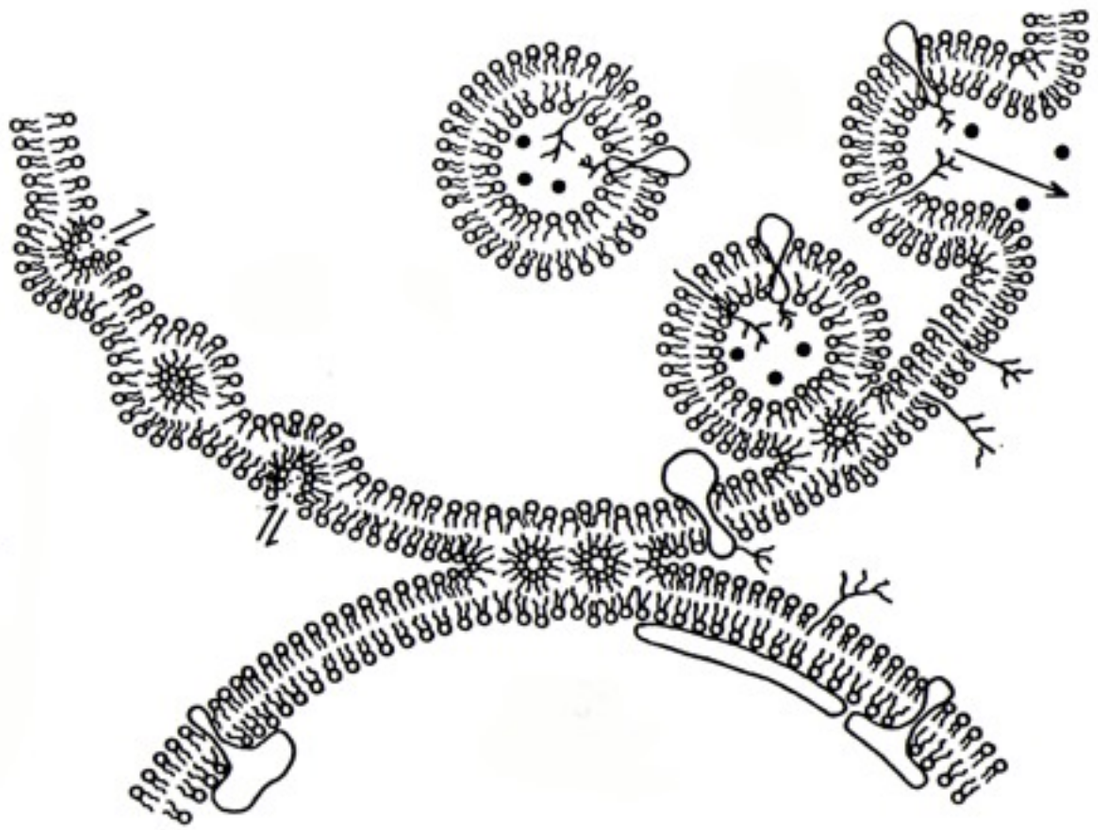
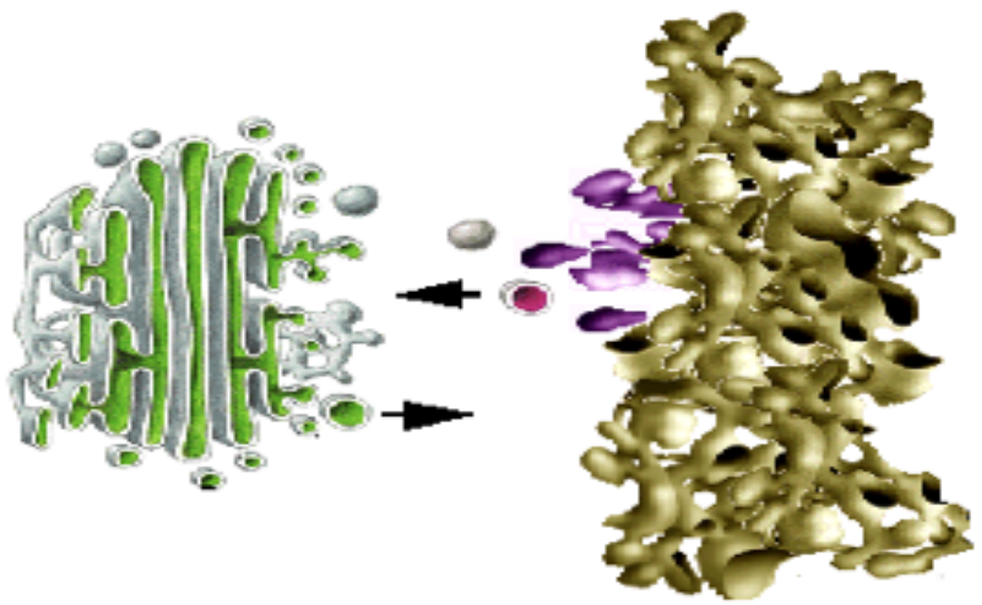


C. K. Haluska et al , PNAS, **103**,15841 (2006)





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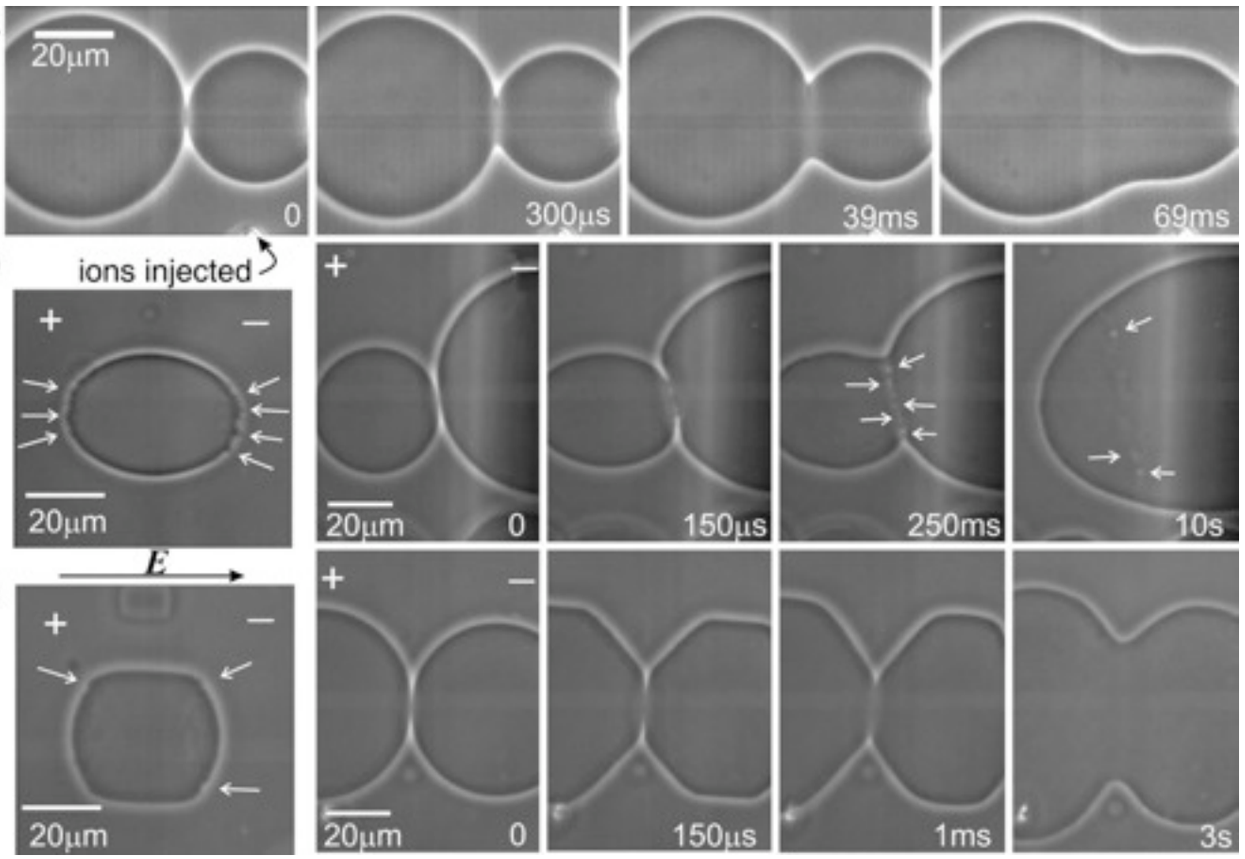

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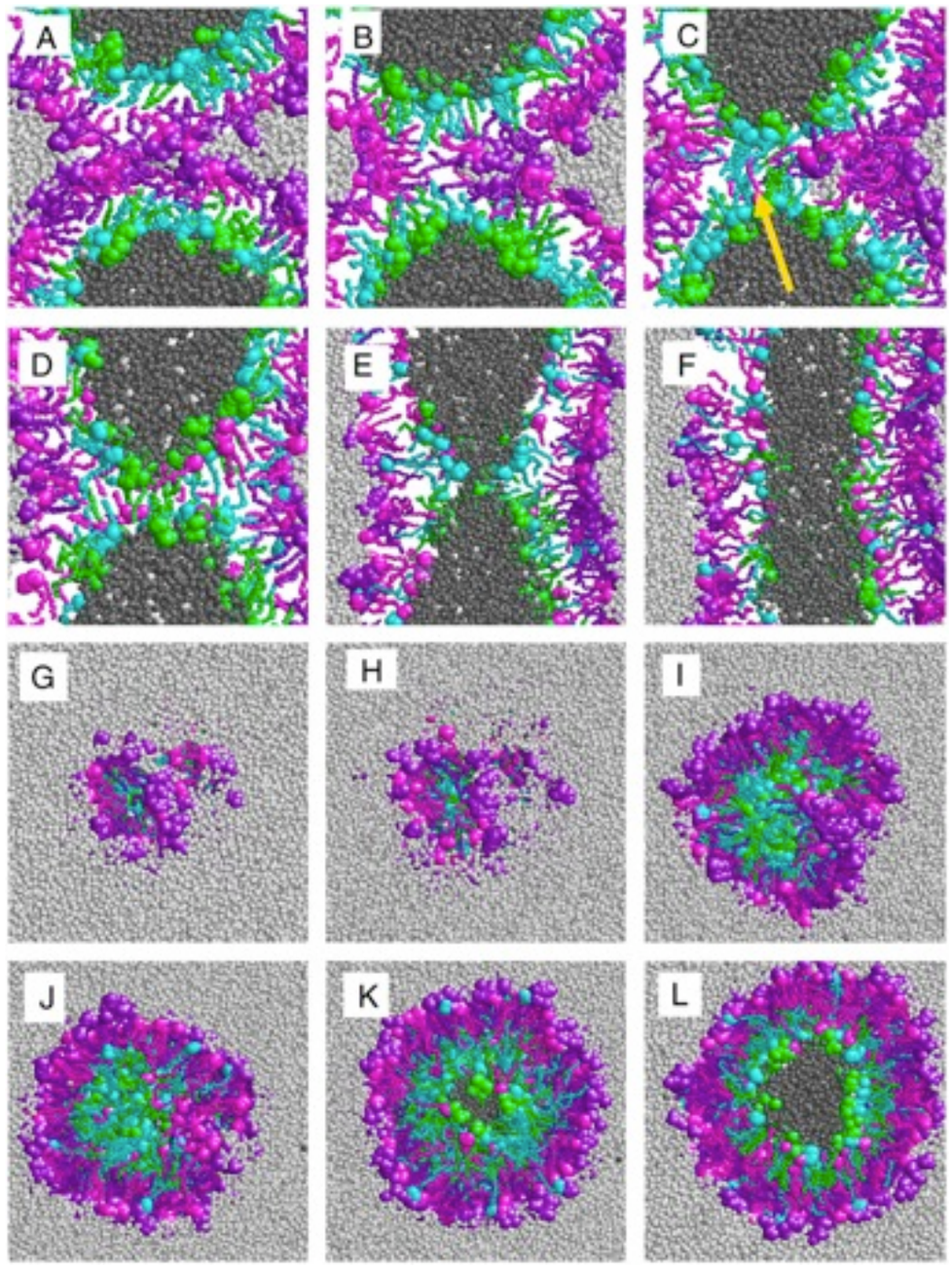

Martini - S. J. Marrink

J. Phys. Chem. B **2007,** *111,* 7812-7824

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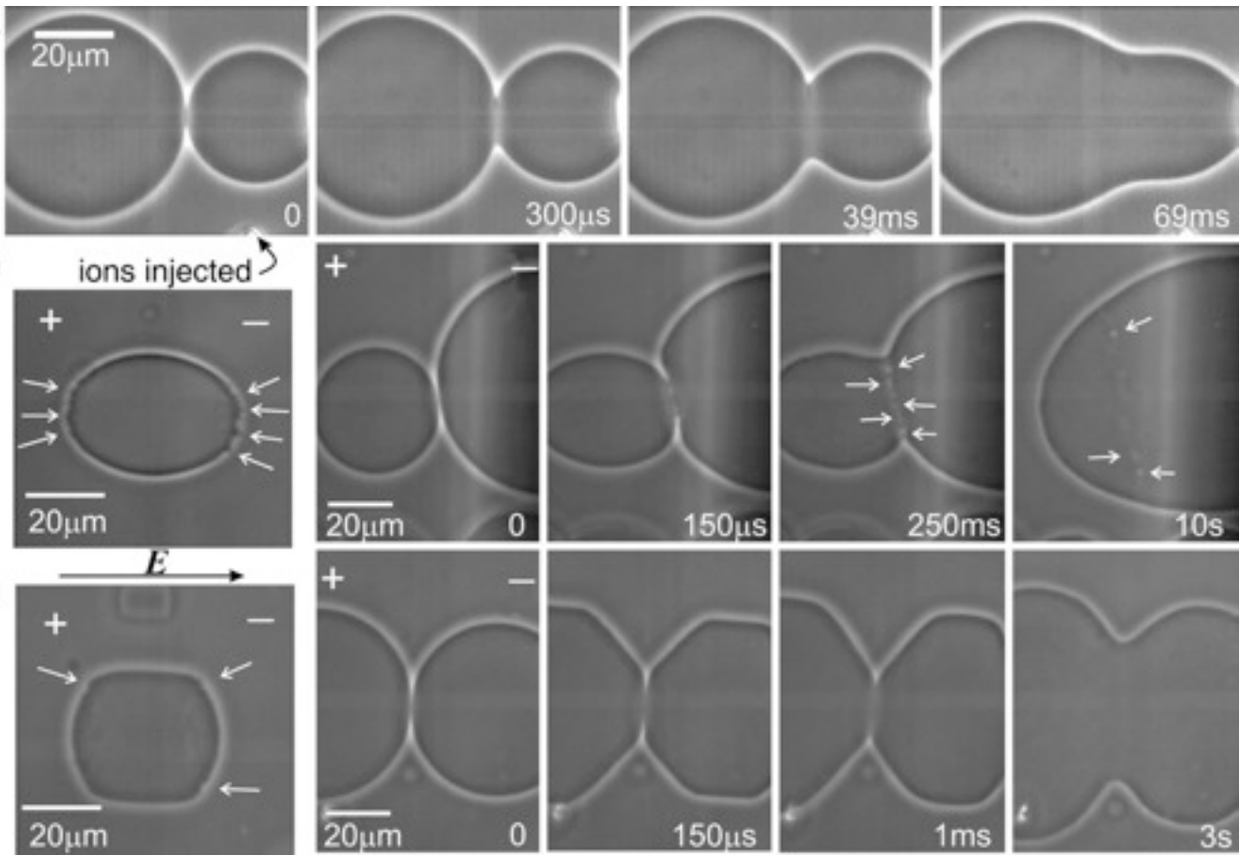

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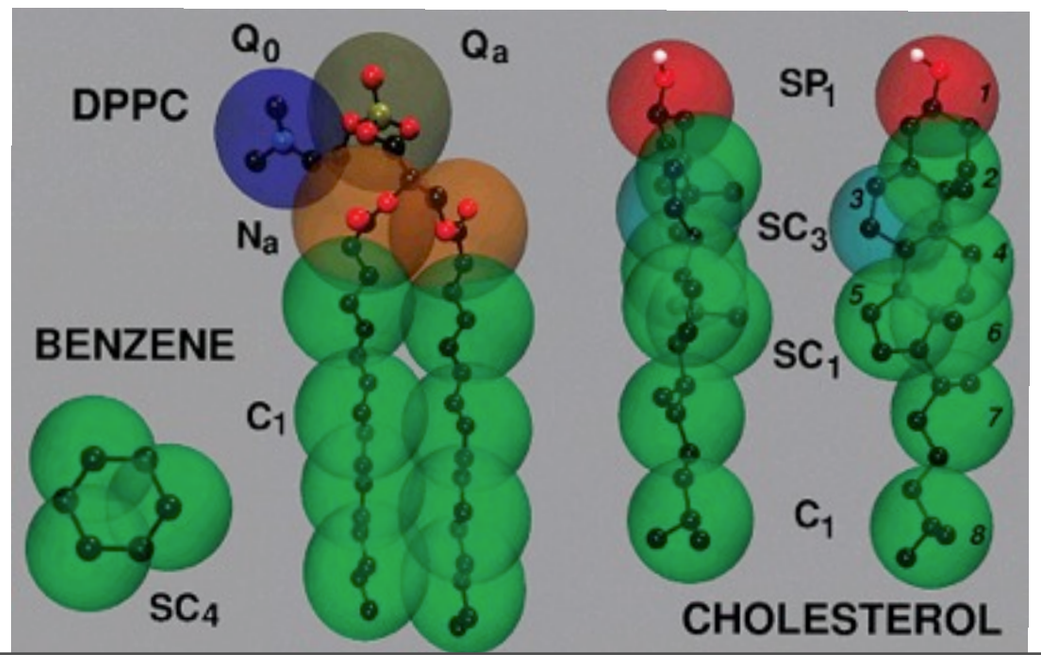

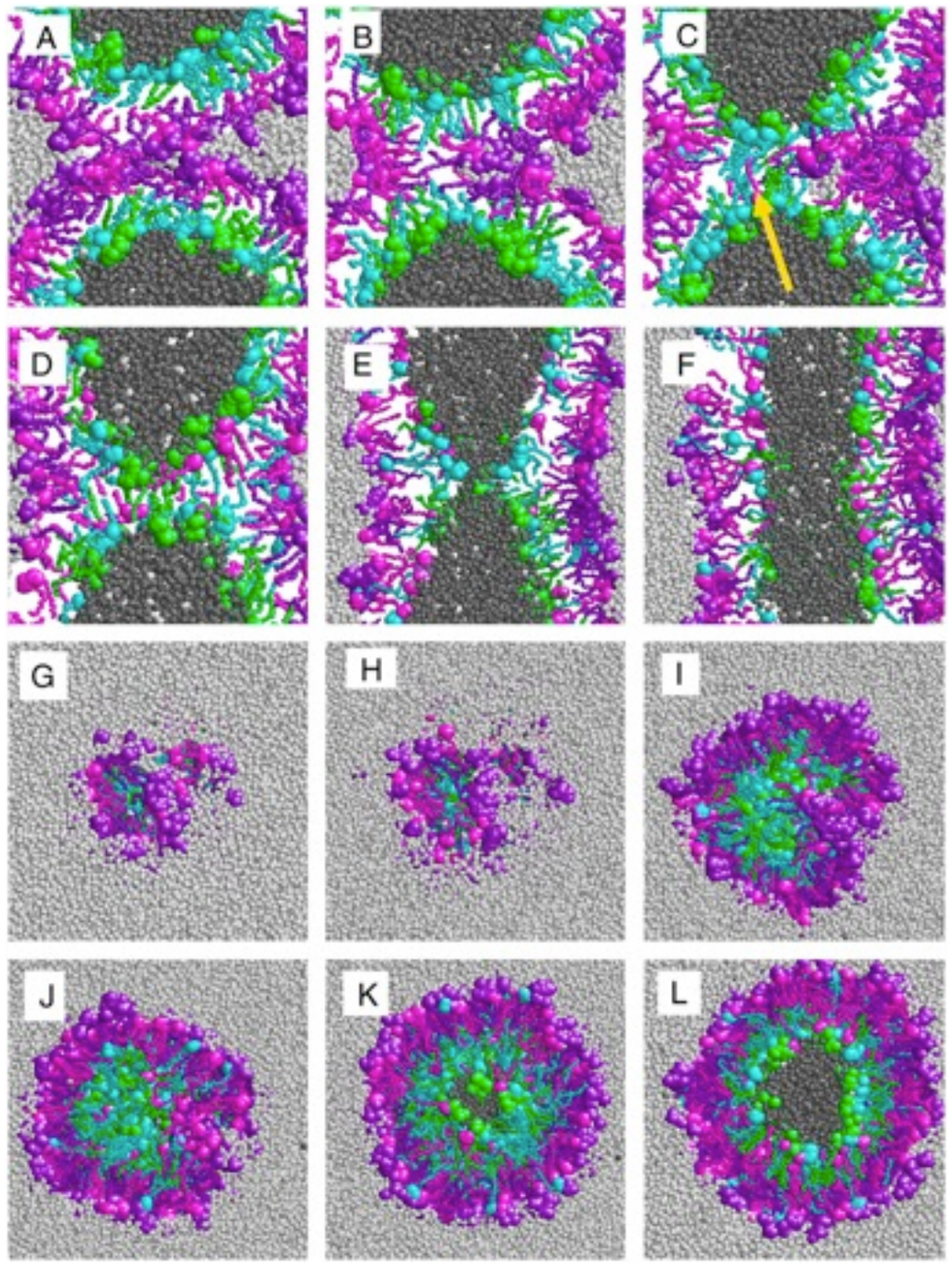

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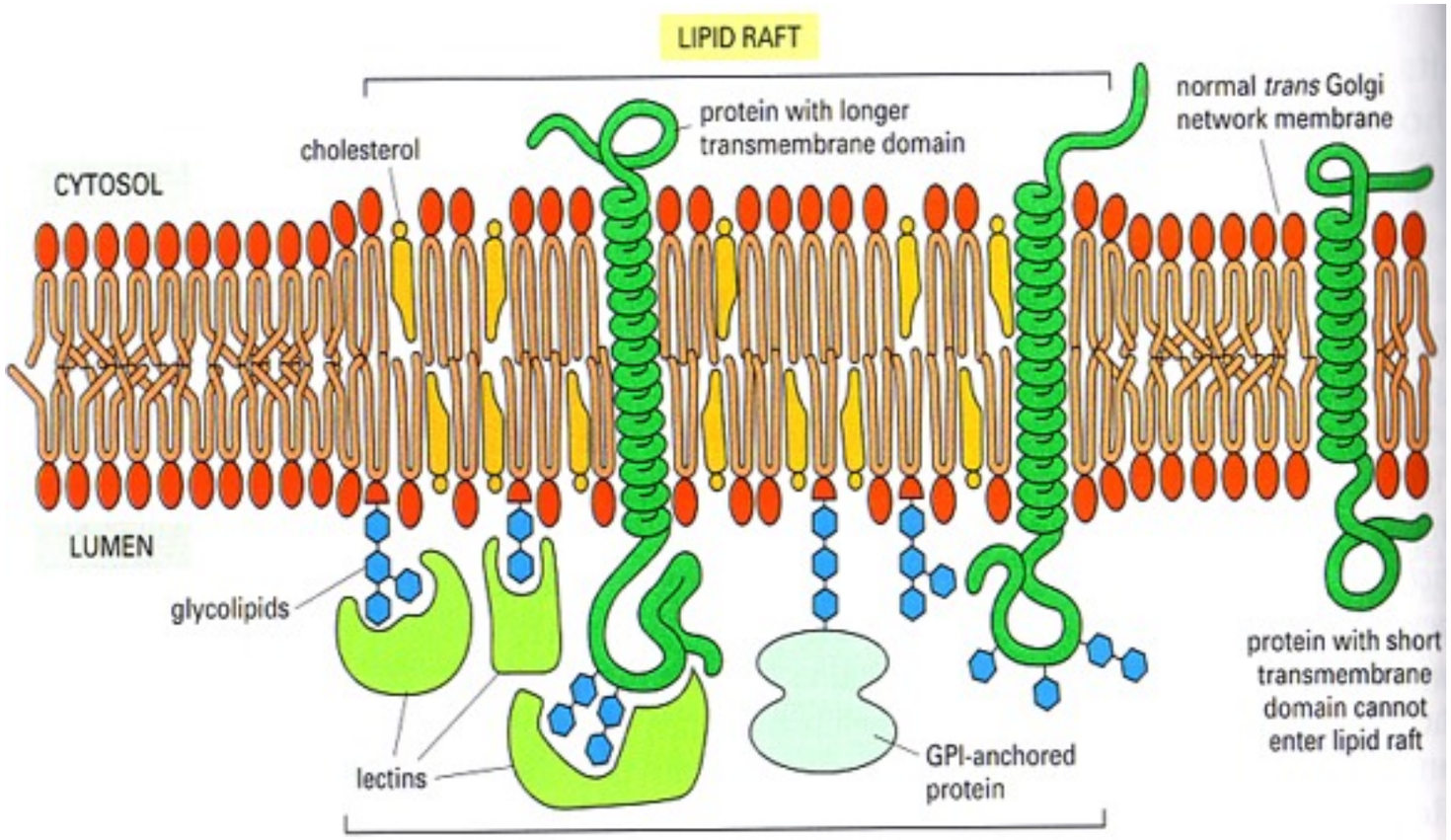
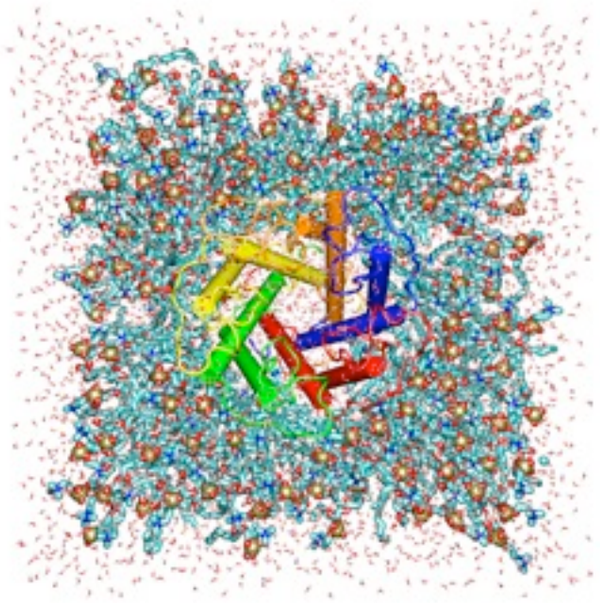
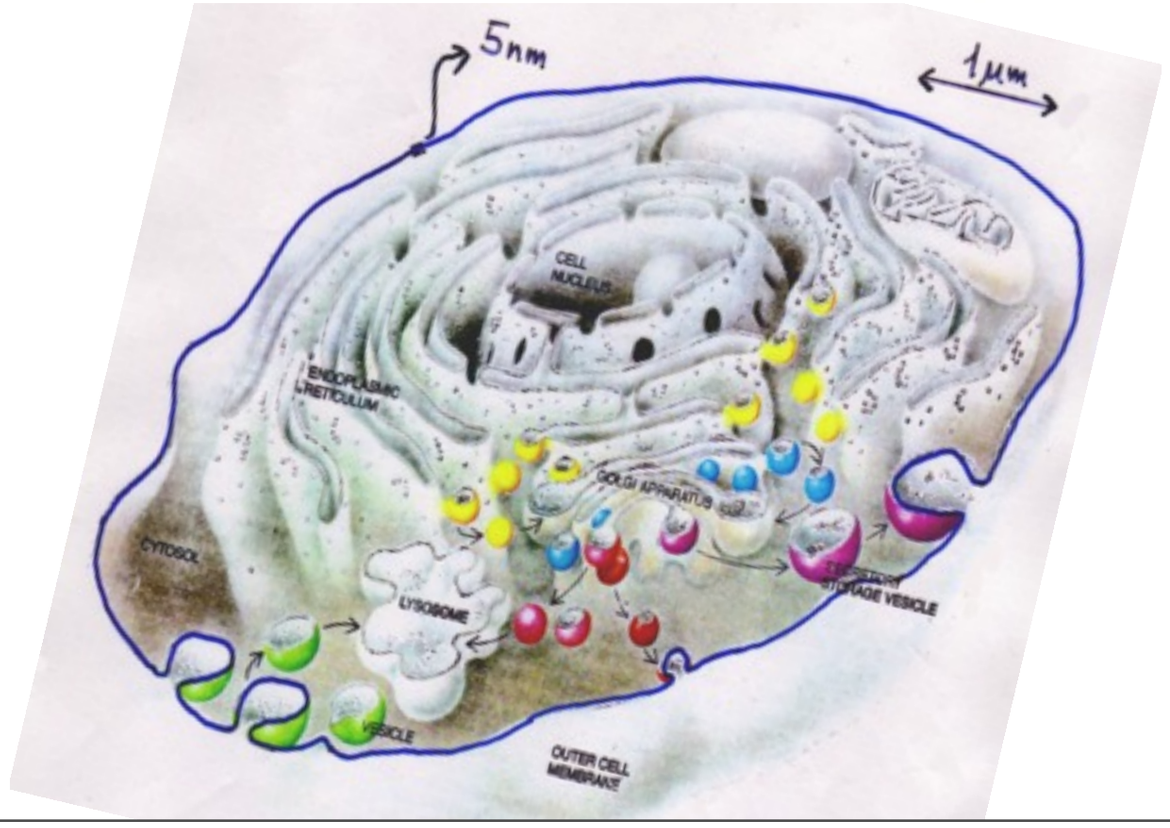
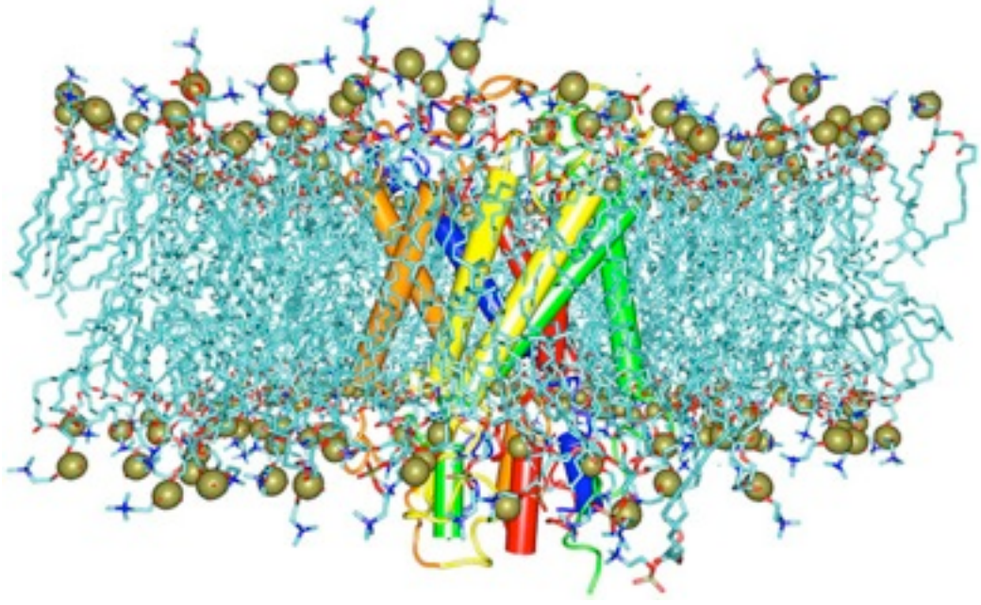
Small-scale membrane structure

Cholesterol, lipid rafts, and hydrophobic matching









Mechano-sensitive channels

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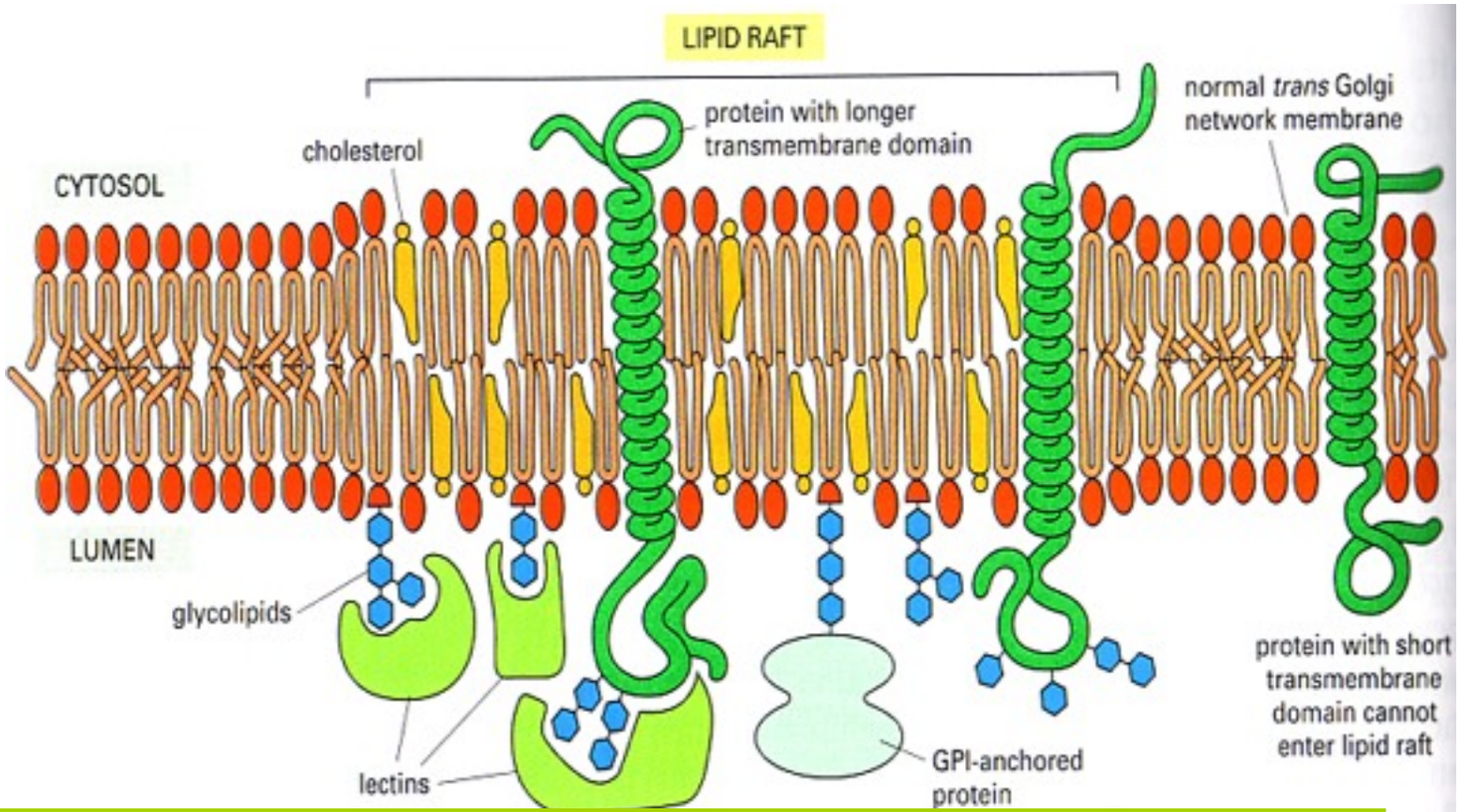
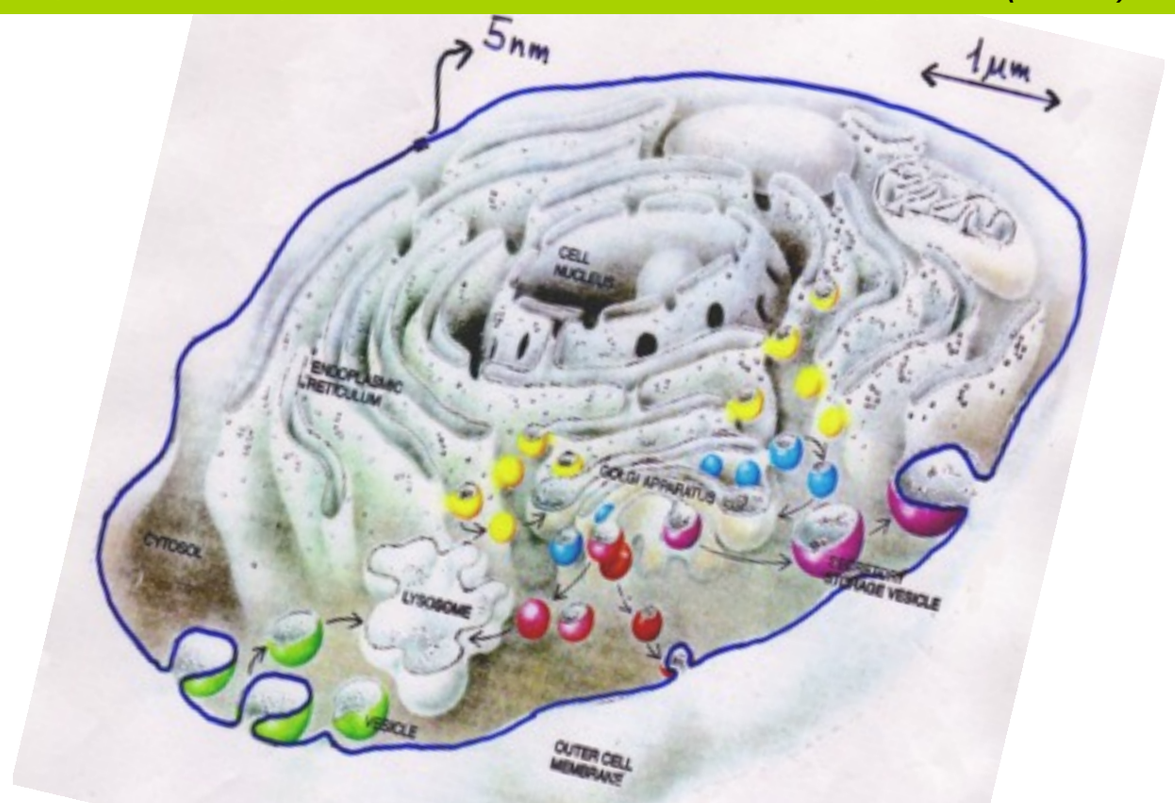
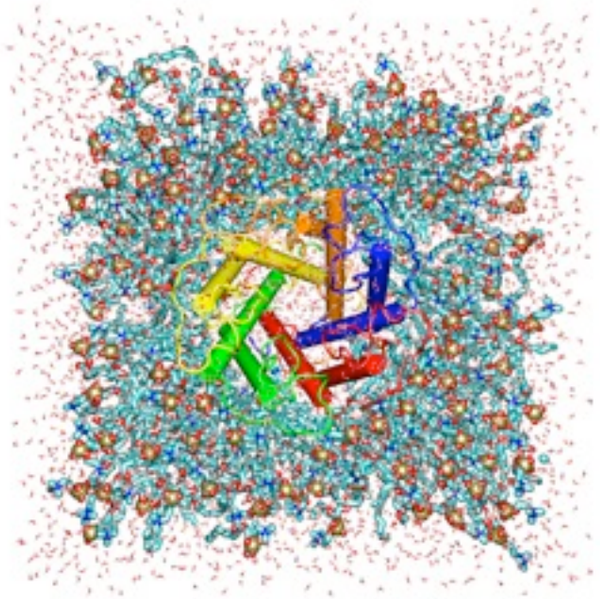
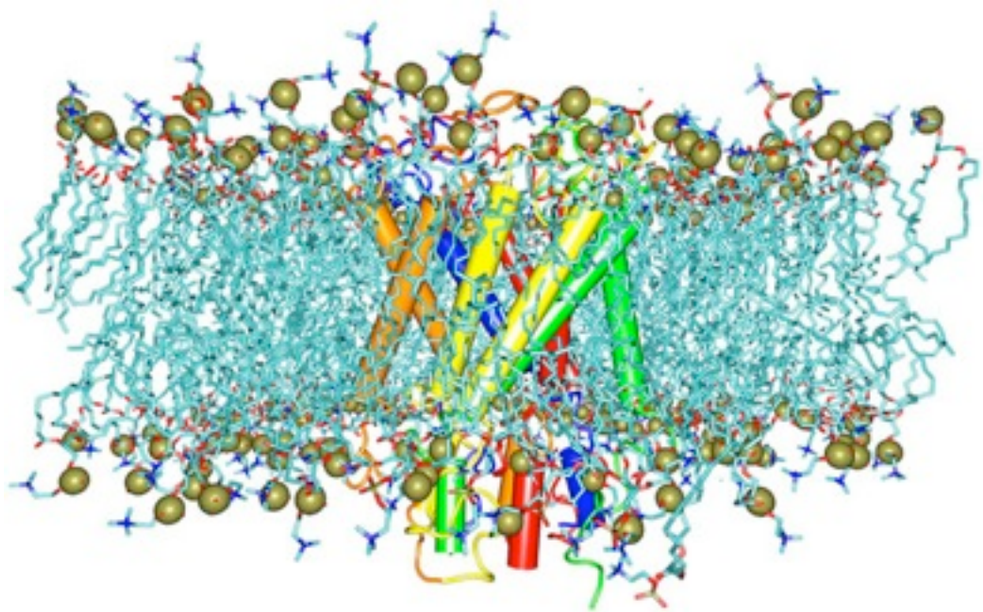


*Jacobson, Mouritsen, Anderson Nature Cell Biol. **9**, 7-14 (2007)*







Mechano-sensitive channels

Coarse graining strategies

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from: *http://www.accelrys.com/technologies/modeling/materials/meso*

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Explicit coarse graining - Clusters of atoms are combined to new entities ("meso-beads")

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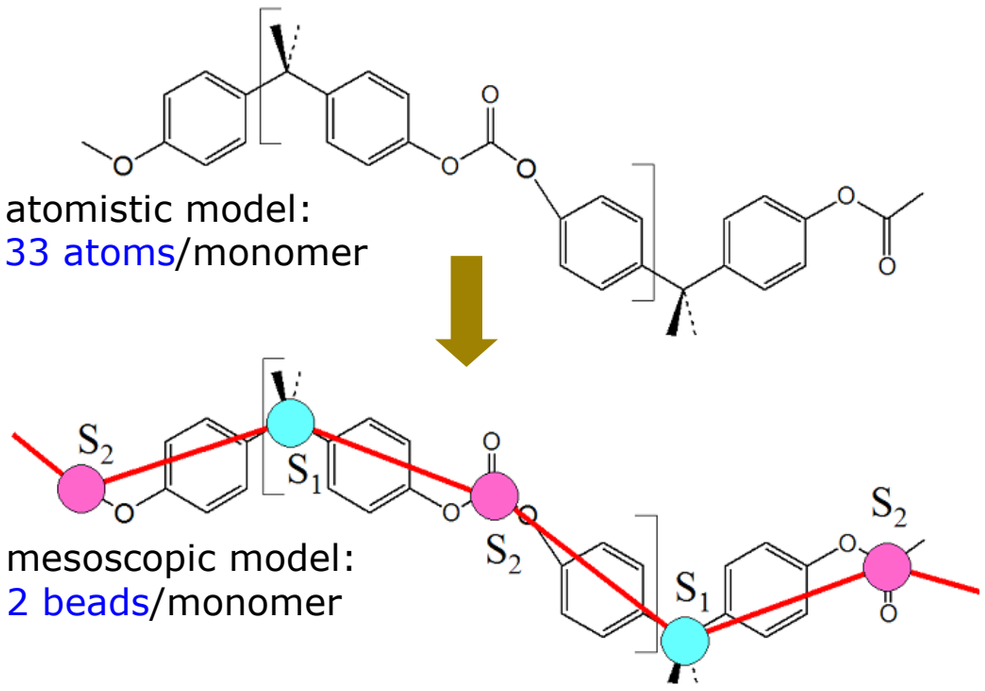
Explicit coarse graining - Clusters of atoms are combined to new entities ("meso-beads")



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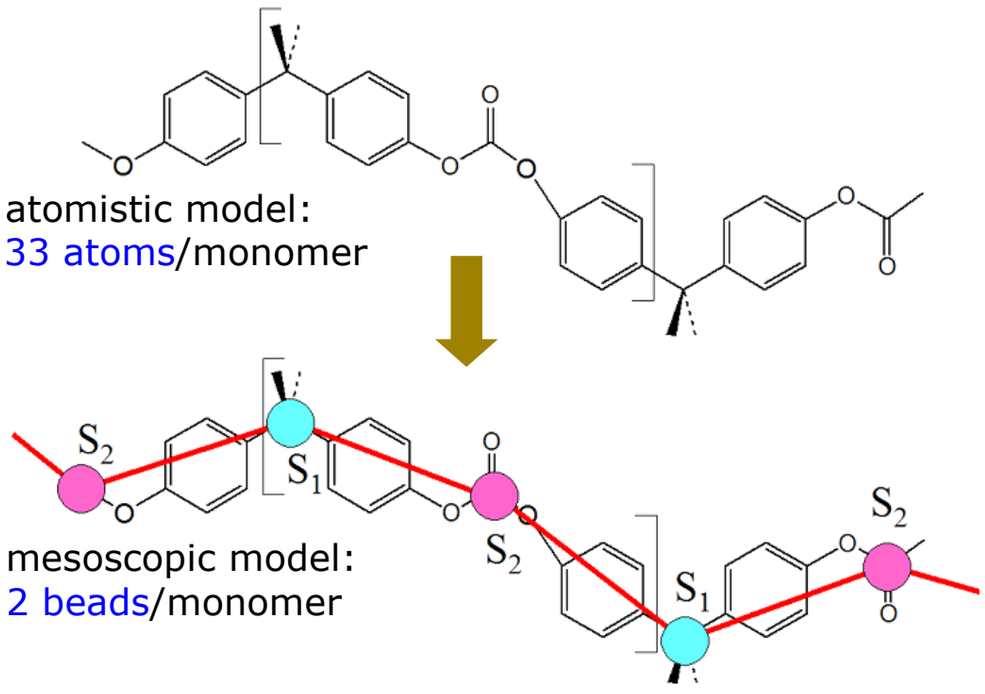

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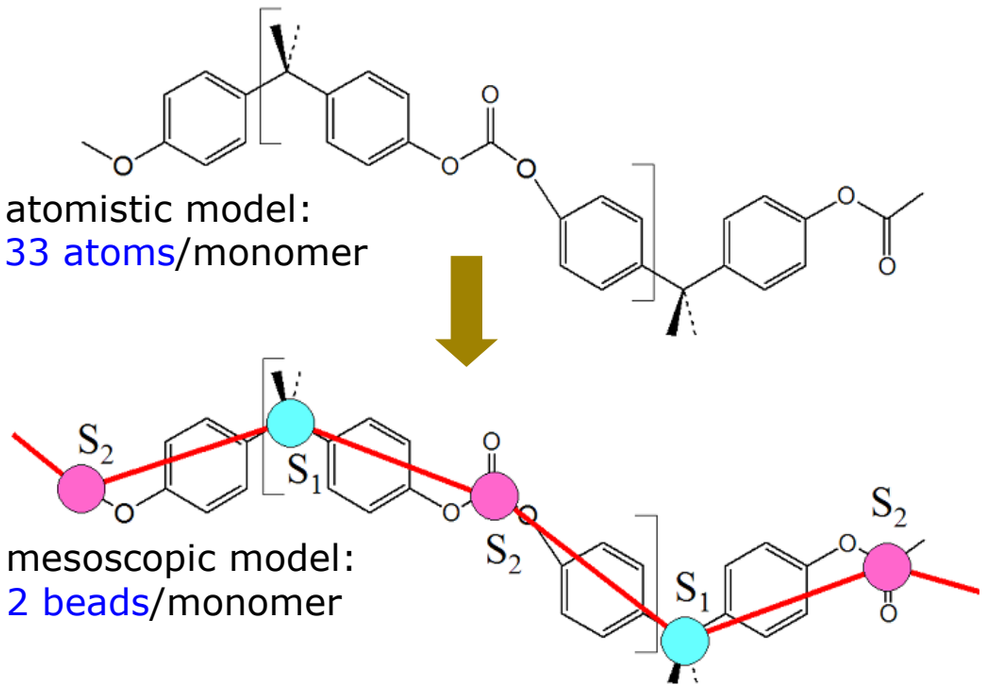

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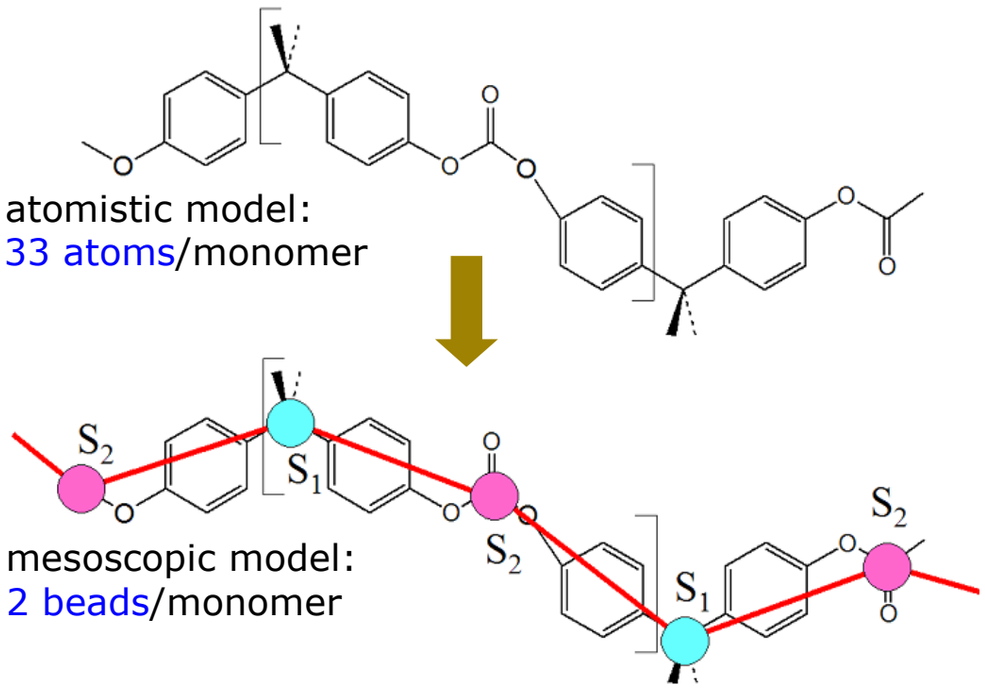

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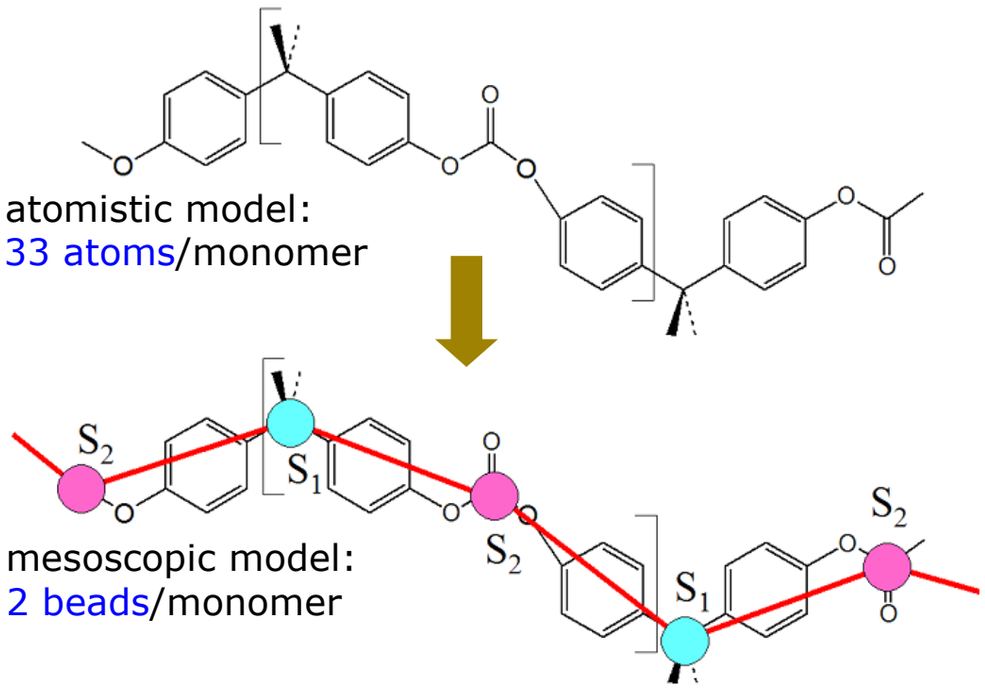

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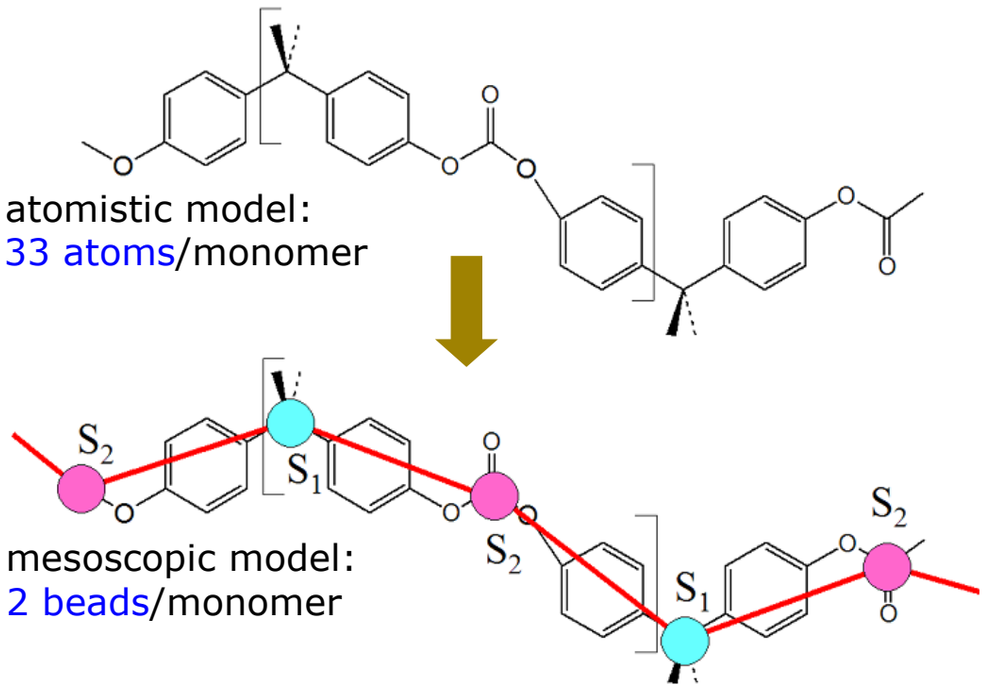

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Adaptive coarse graining - Delle Site

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Amalendu Chandra and Marcus Elstner

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Maddox, J. Crystals from first principles. *Nature* ***335, 201–201 (1988).***

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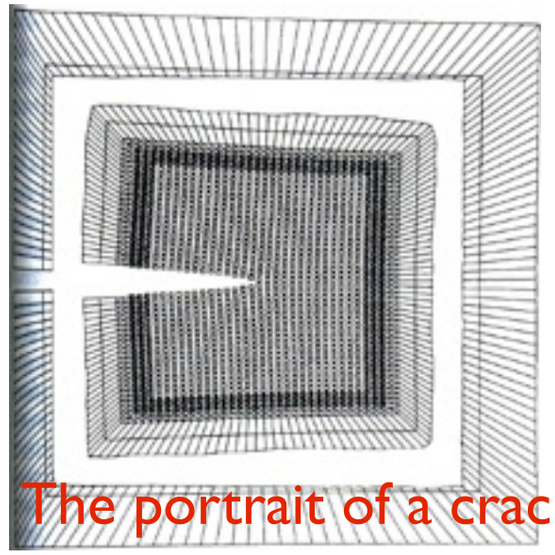

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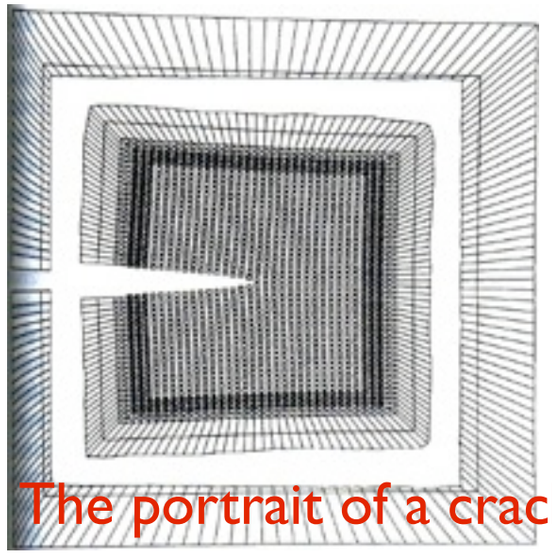

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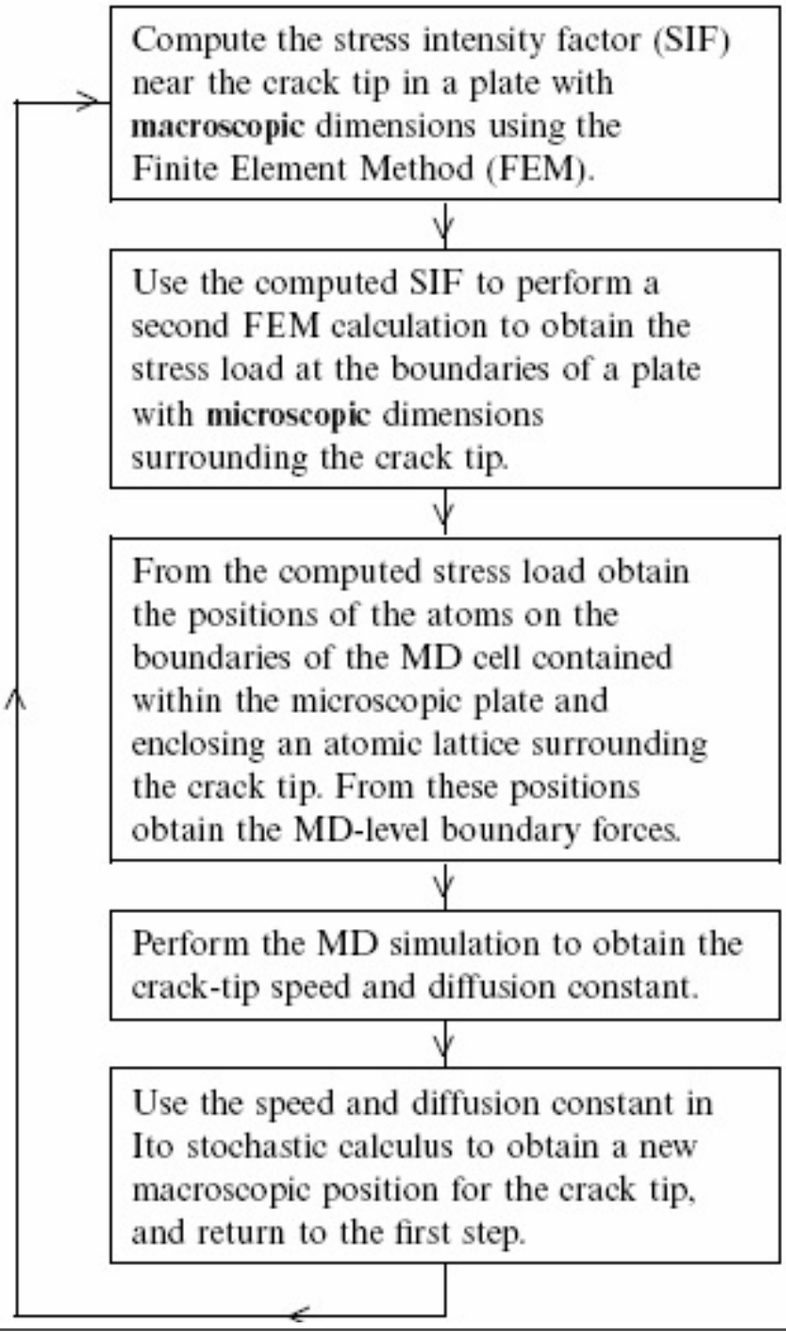

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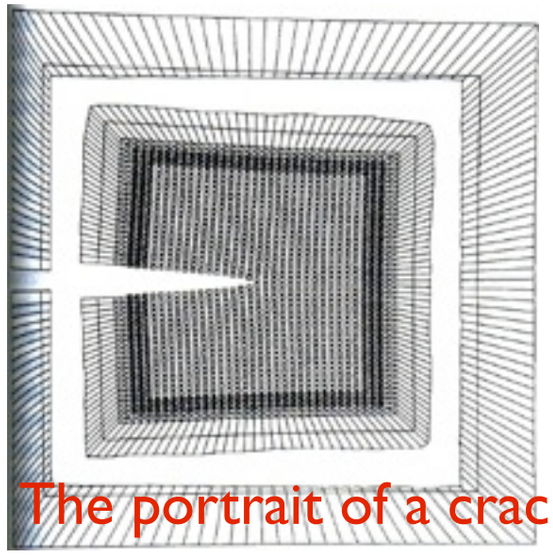

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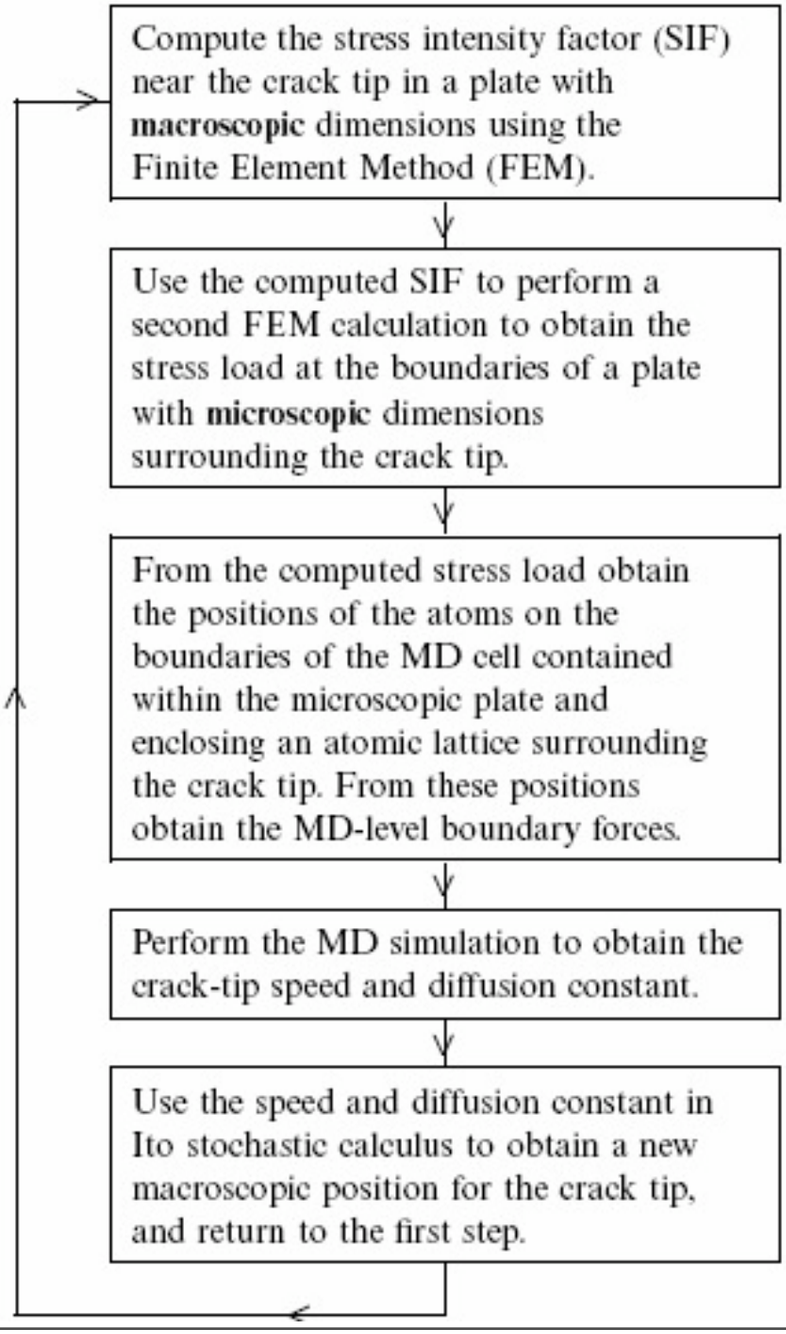

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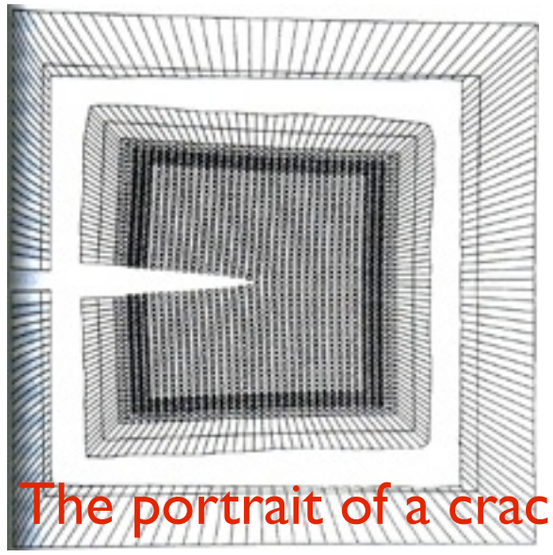

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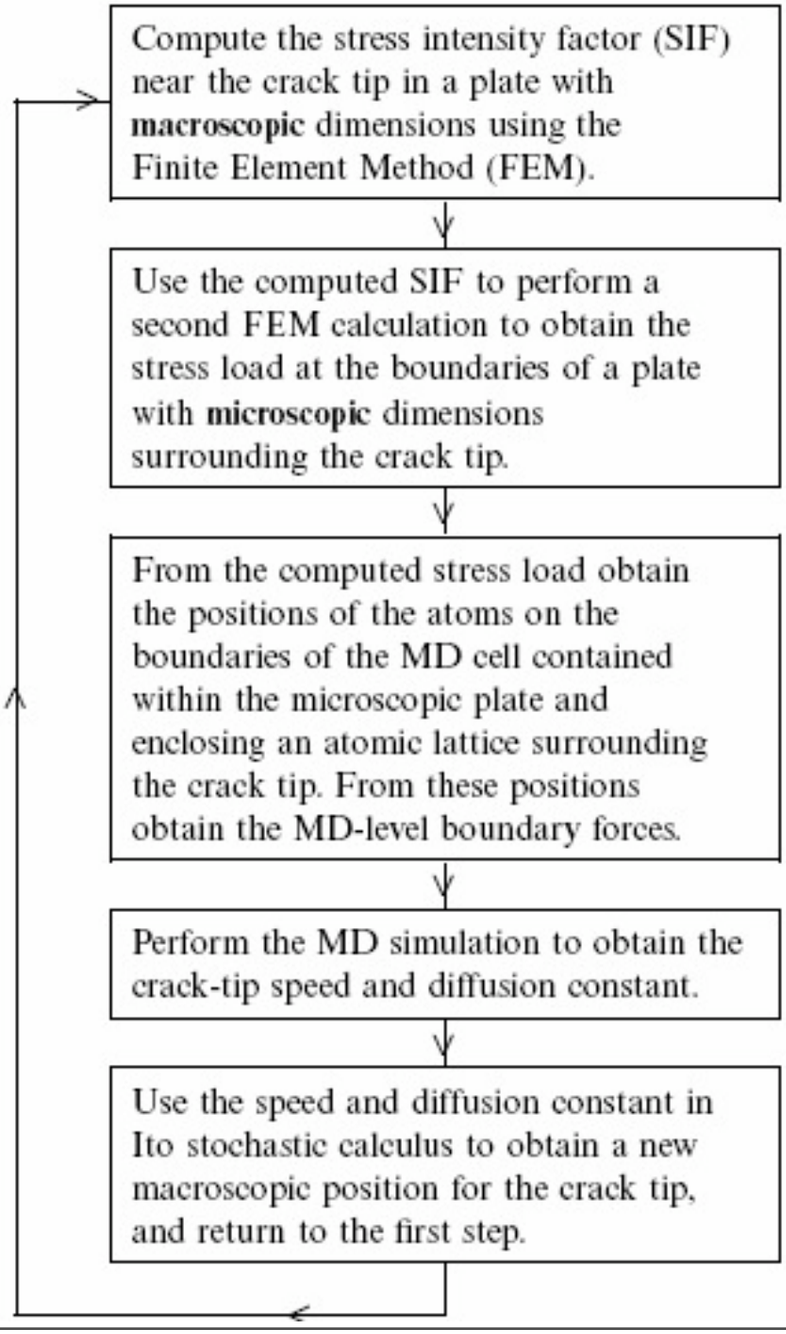

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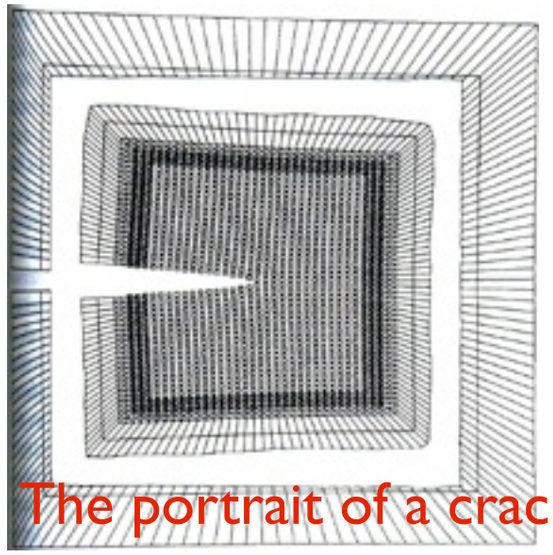
•One strategy is to determine the properties of the dislocations using atomic level details and feed this information to a dislocation dynamics simulations in which the basic units are dislocation interacting though the strain fields. The results from this calculation is then used to determine the material/device properties.



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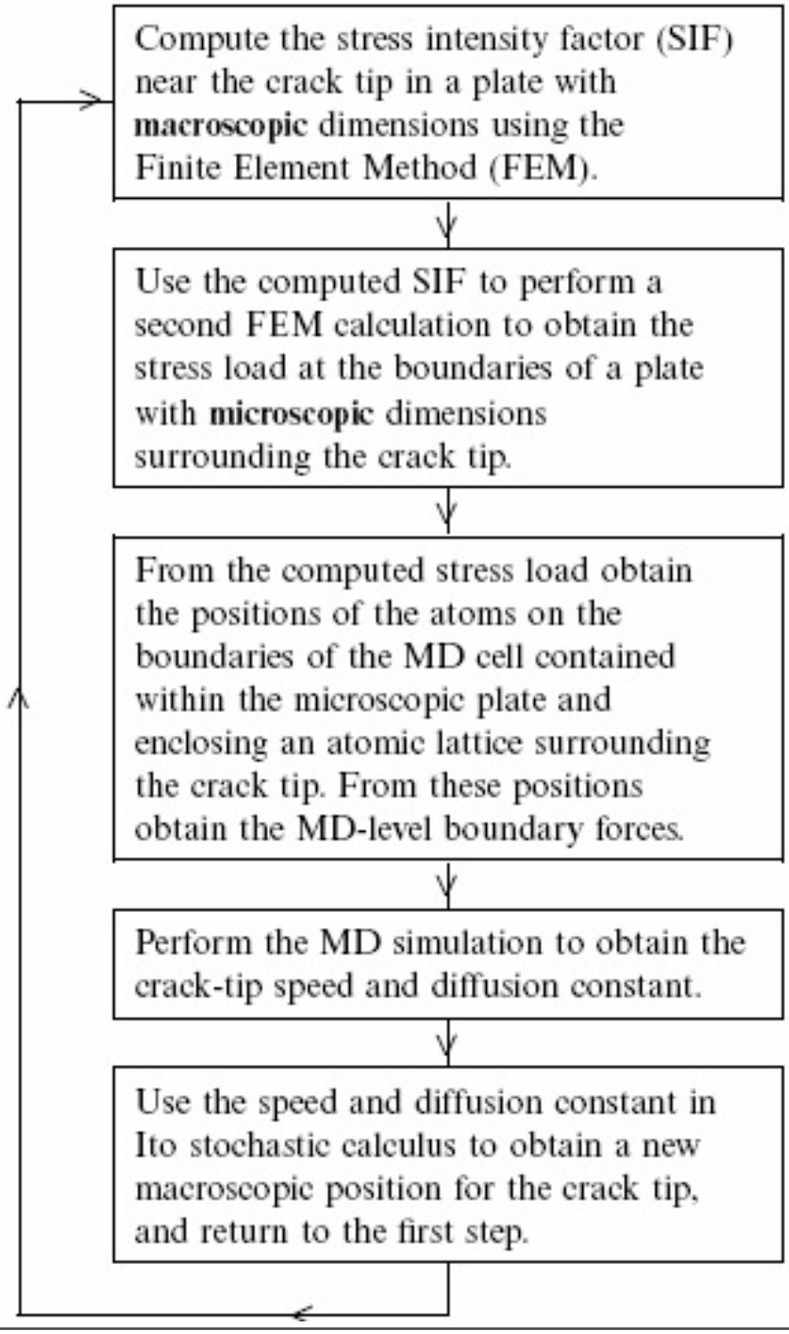


Hard materials Multiscale Strategy

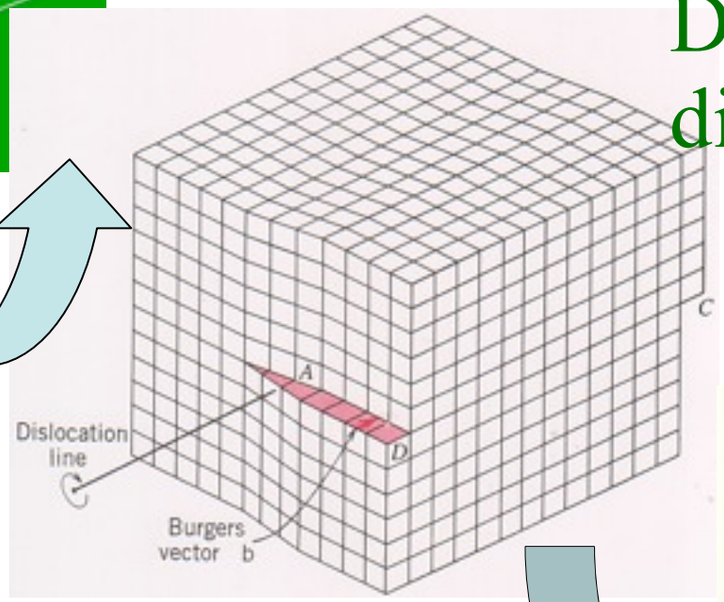
"First-principles" or "*Ab Initio*"

Electronic orbitals,
Nuclei, vibrations

Material-specific
microscopic info

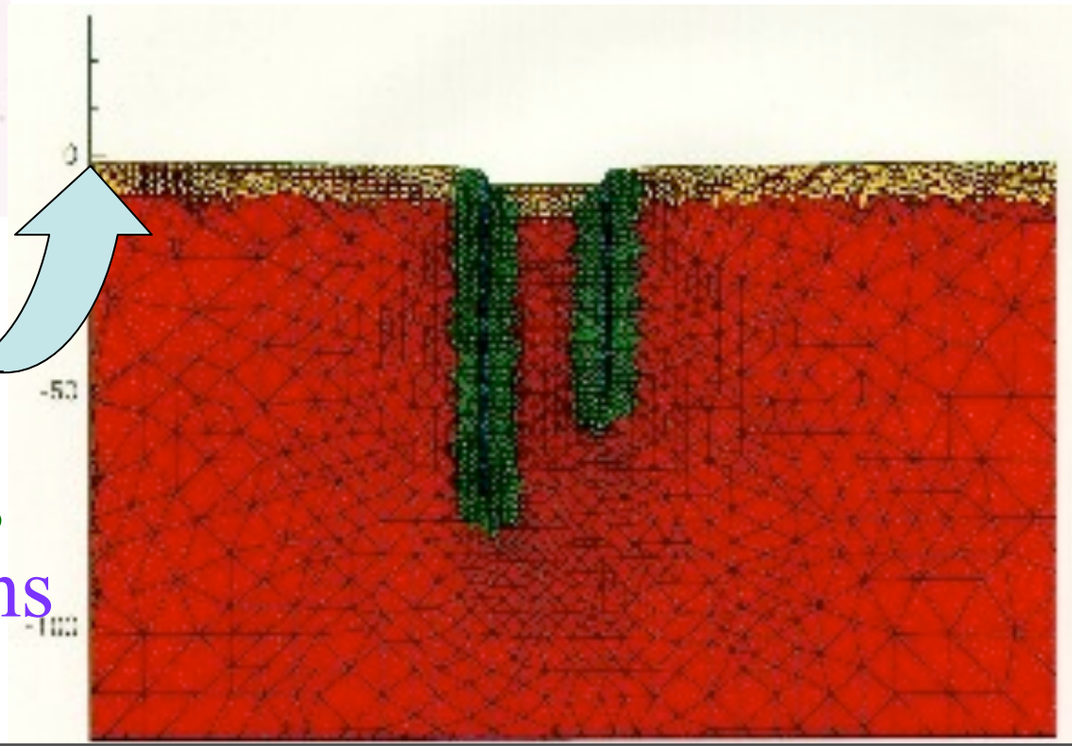
Sub-angstrom

Defects, e.g.. grains,
dislocations



Intermediate-scale
structure: properties

Nano-m, microns



μ, mm

Continuum analysis
Devices, applications

Landau-theory

Ab Initio Approaches

Electronic Problem: First-principles Methods
(Density Functional Theory)

Symmetries → ← Microscopic Picture:
Bonding, Couplings, Instabilities

integrate out DoF

Ab Initio Modeling

H_{eff} : Effective Hamiltonian (model)
Focus on relevant phase subspace

eg. Ising, Heisenberg Lattice Dynai

Energy, forces

Ab Initio MD, Monte Carlo

Simulations MD, Monte Carlo, FEM

Macroscopic, T ≠ 0 Response,
Different length Scales phenomena
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Limitations of Ab Initio to FEM , Constitutive multiscale modeling - Michale Falk

Topics in hard materials: multiscale phenomena

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- Collosal magneto-resistance materials: many energy-scales