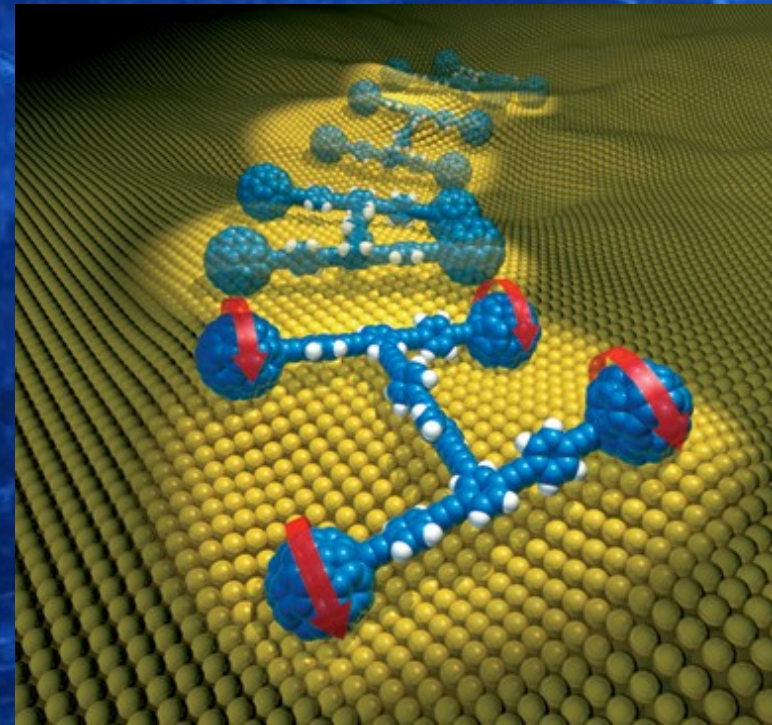


Student Colloquium: Simulation of carbon nanotubes and membranes

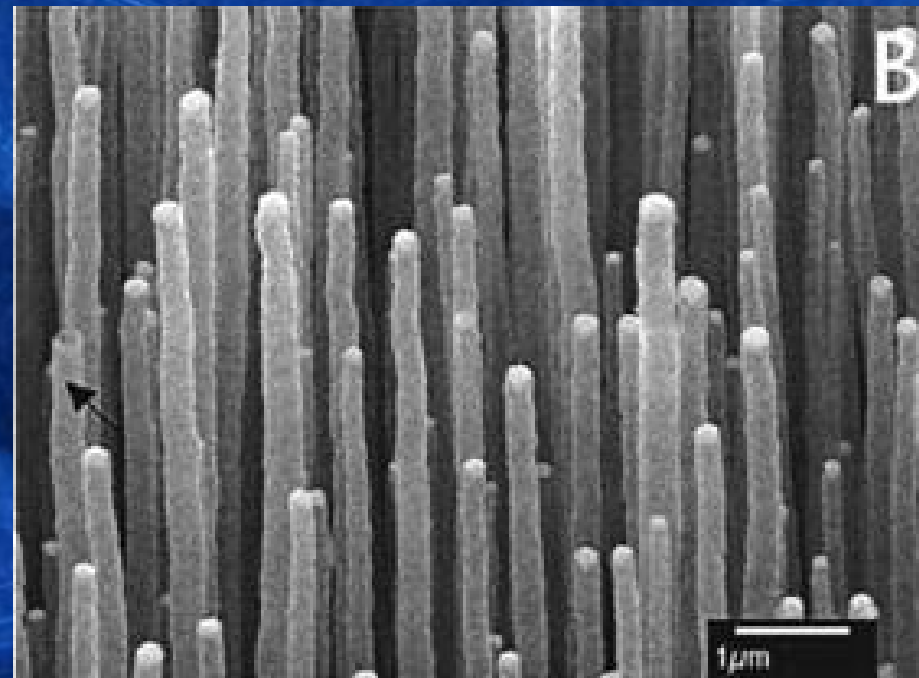
Student:
Supervisor:
01-05 / 15-06

Danny Arends (s1276891)
Prof. S.J. Marrink



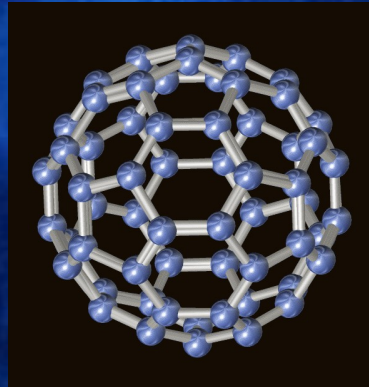
Overview

- Introduction fullerenes and nanotubes
- Short history
- Production & properties
- Simulations
- Concluding remarks



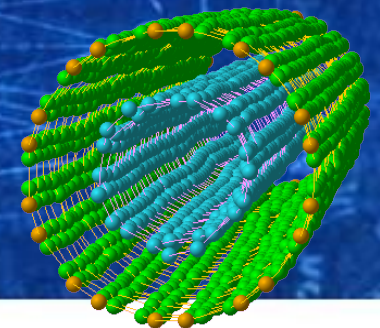
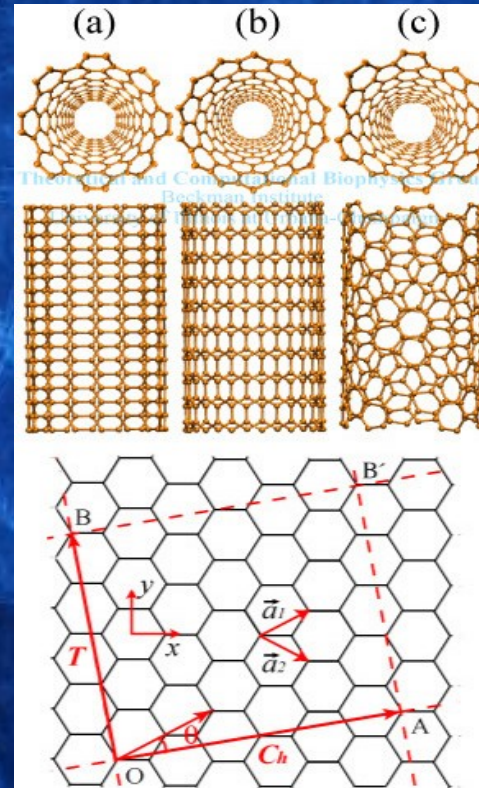
Nanotubes and fullerenes

- Fullerenes



- Single-wall nanotubes

- Double-wall nanotubes

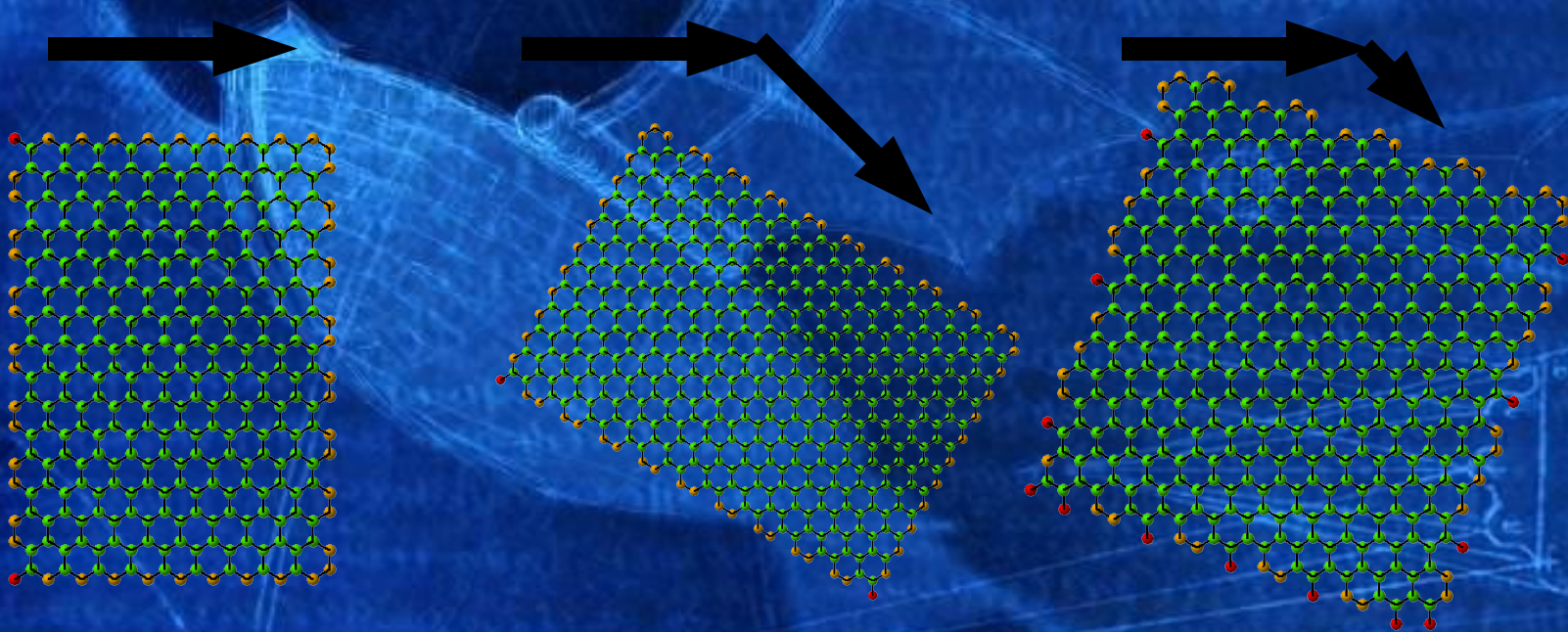


Single-Wall Nanotubes

- ZigZag
- 10,0

Armchair
10,10

Chiral
10,5



History

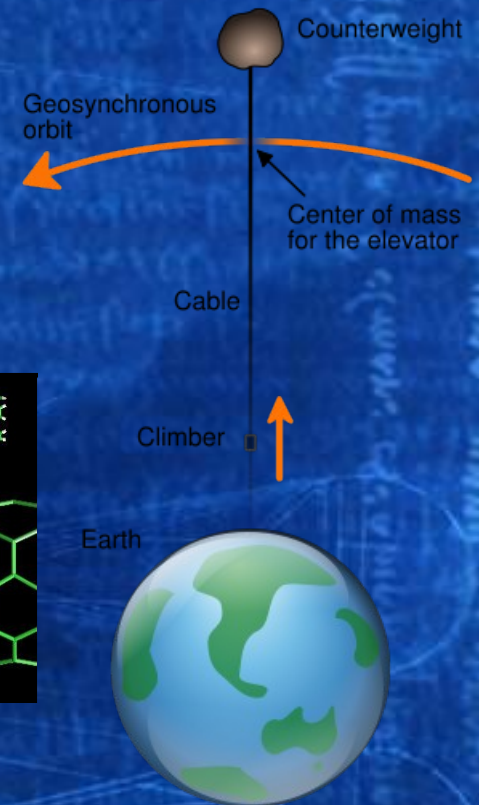
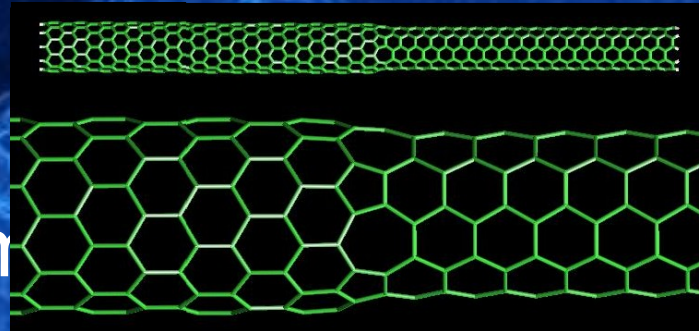
- 1100-1700 Damascus steel
- 1802 Arc discharge
- 1898 Rediscovery (Edison)
- 1952 Image of MWNT
- 1991 Iijima
- 1996 Nobel prize C₆₀ fullerene
- 1999 First storage of hydrogen in SWNT
- 2001 Super conductive SWNT
- 2006 Nanoparticles and prostate cancer
- 2008 Production of hybrid silicon / SWNT



Image from: damascus.free.fr

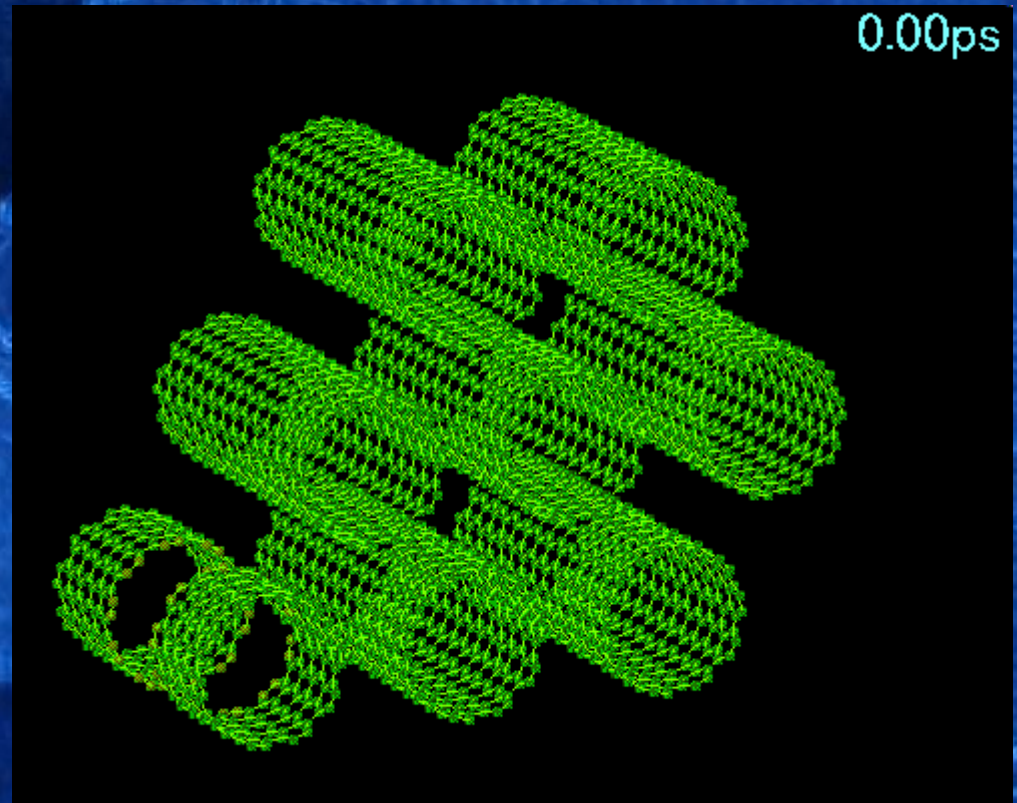
Properties of Nanotubes

- Mechanical Strength
- Electrical properties
- Optical activity
- Pore formation in n



Simulation of storage capacity

- Single wall nanotubes storing hydrogen
- Storage/Weight



(1) Image from: <http://www.photon.t.u-tokyo.ac.jp/~maruyama>



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groningen



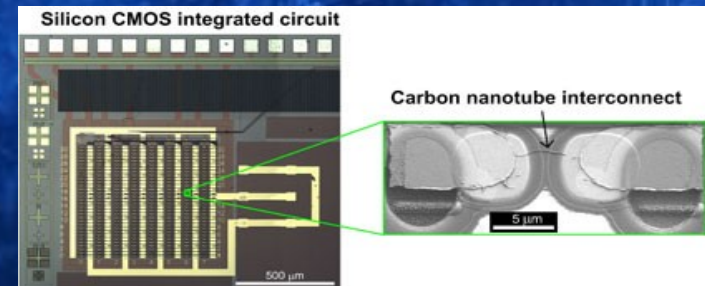
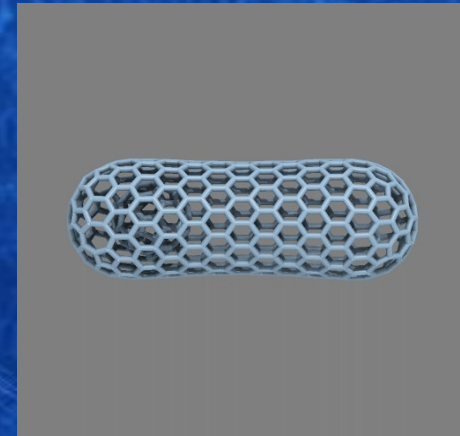
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The MD Group

Molecular & Mesoscopic Dynamics in Complex Systems

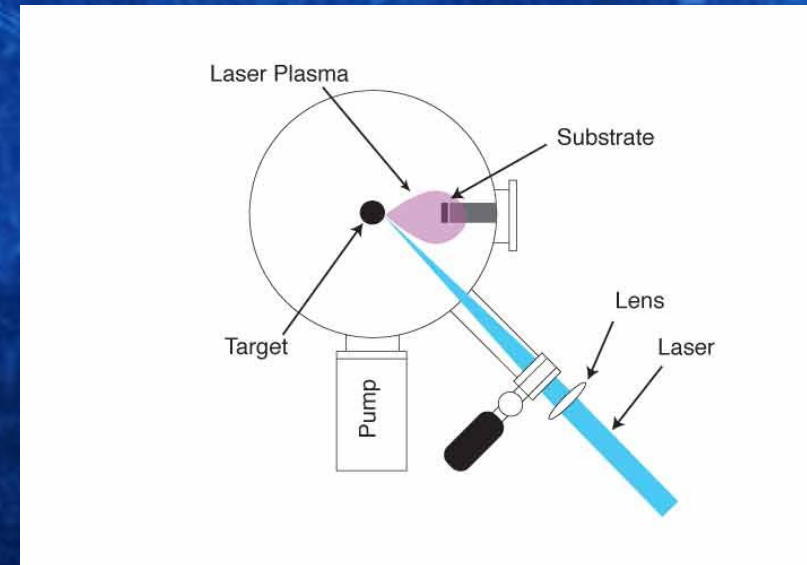
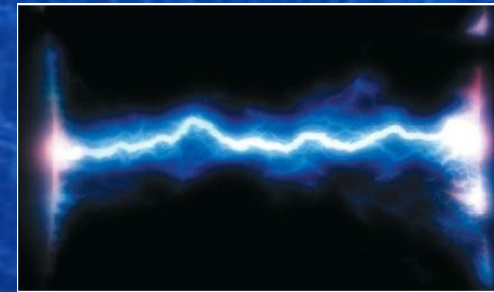
Simulation of computer components

- Metallic or semi conducting
- Nano scale memory
- Single wall nanotube



Productie Nanotubes

- Production methods
 - Arc discharge
 - Laser ablation
 - Chemical vapor
 - (Flame synthesis)



Long term goals

- Drug targeting
- Antibiotics
- Hydrogen storage (fuel cell)
- Nanoscale transistors
- Nanoscale probes/sensors
- Portable X-ray devices

Membranes

- Maintains cellular stability and integrity
- Protective and selective barrier
- Controls and directs cellular activity
- Complex environment
- Simulation using martini lipids

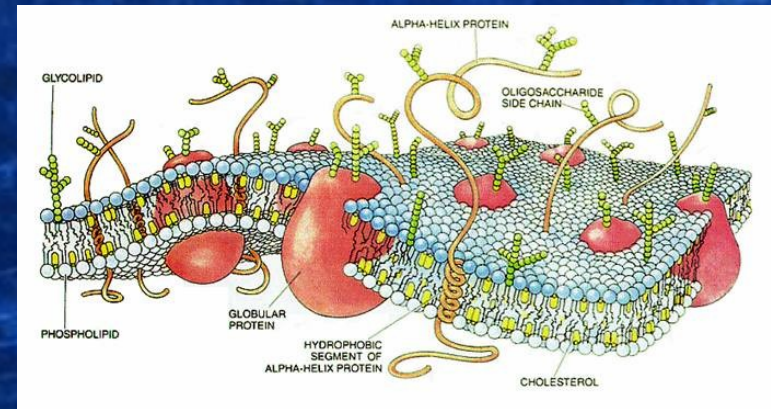


Image from: wikipedia.org

Nanotubes and membranes

- Toxicity
- Diameter of the tube
- Shape of the tube
- Tube with functional groups
- Model for pore formation

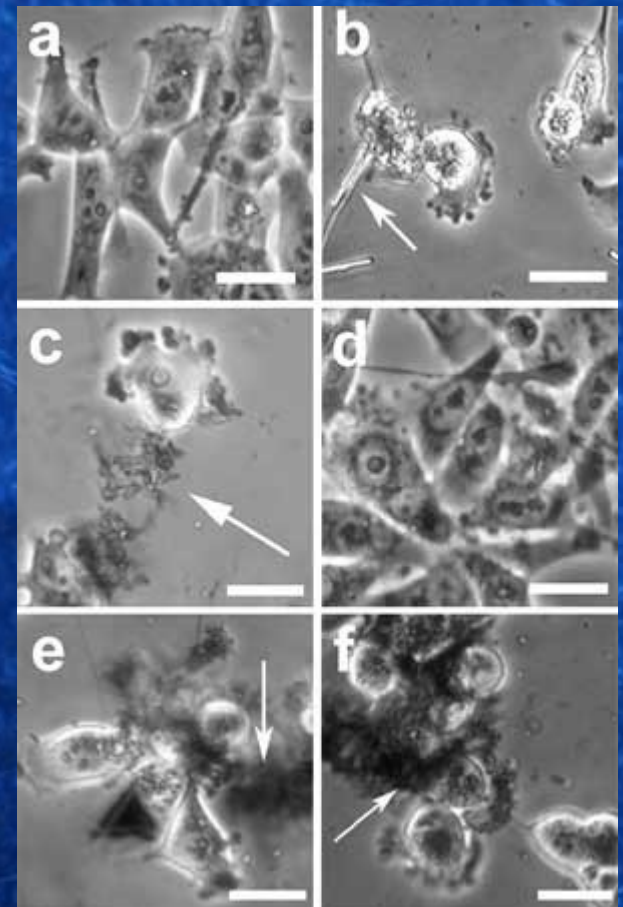


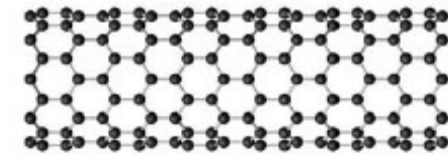
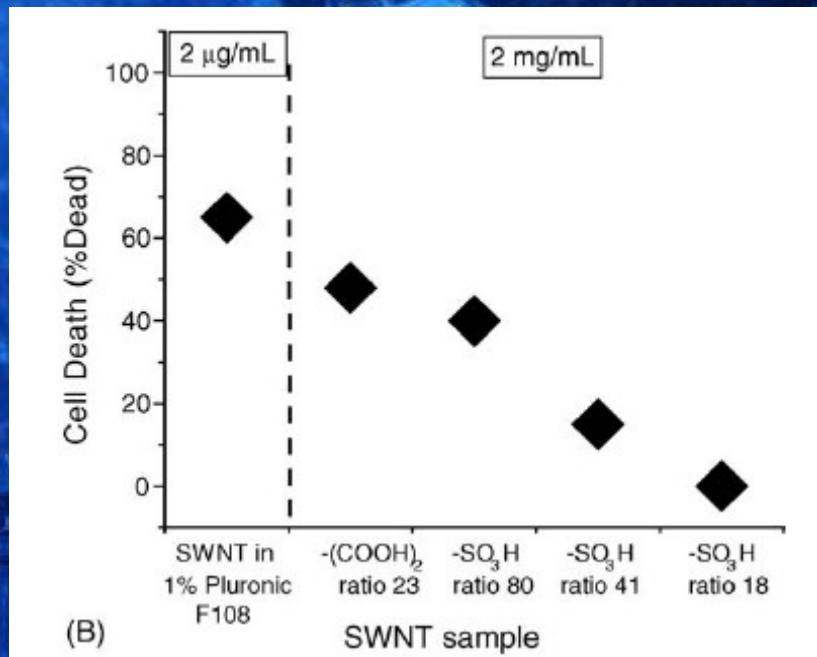
Image from: www.nanowerk.com

Lam CW, James Jlt et al. "Pulmonary toxicity of single-wall carbon nanotubes in mice 7 and 90 days after intratracheal instillation." *ToxSci Advance*, 2003.

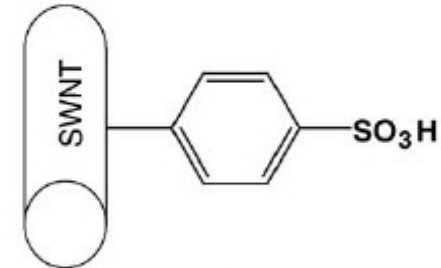
Collaboration of German&Swiss universities

Reducing toxicity

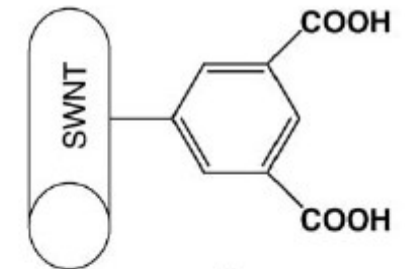
- Adding coating material
- SWNT vs MWNT



SWNT



1



2



Simulation

- Setup initial state
- Calculate forces on particles
 - Short range interactions (VDW)
 - Long range interactions (Charged particles)
- Move particles

Simulation

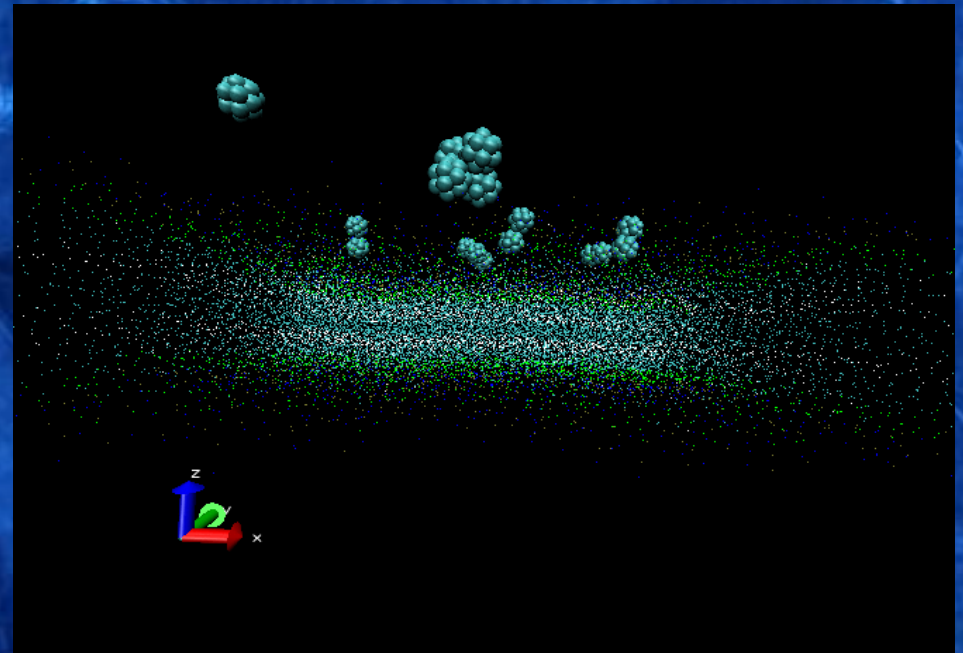
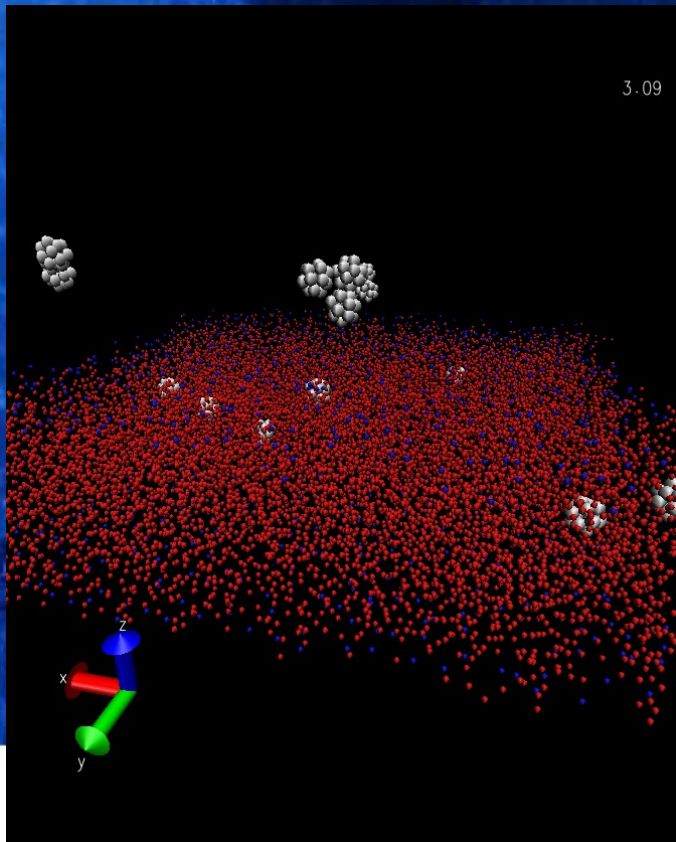
- Packages available: GROMACS, NAMD
- Classical MD
 - Timescale problems
- Coarse grained MD
 - Less detailed
 - Larger timescale or system

Simulation

- Fullerene particles and DOPC membrane
 - Coarse grained
 - Martini force field
 - Martini lipid DOPC
 - Additional parameters for nanotube particles from literature

Simulation

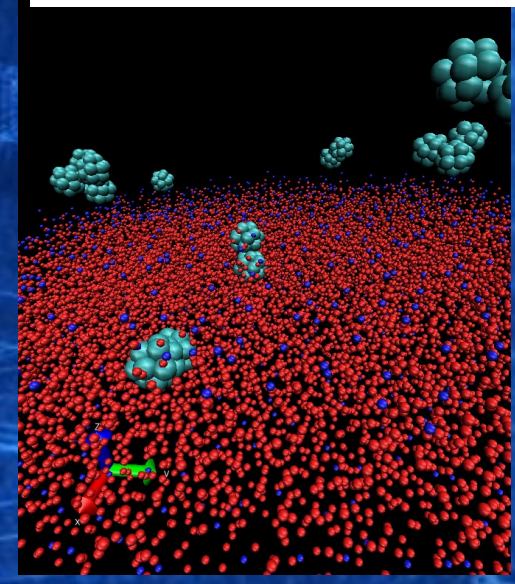
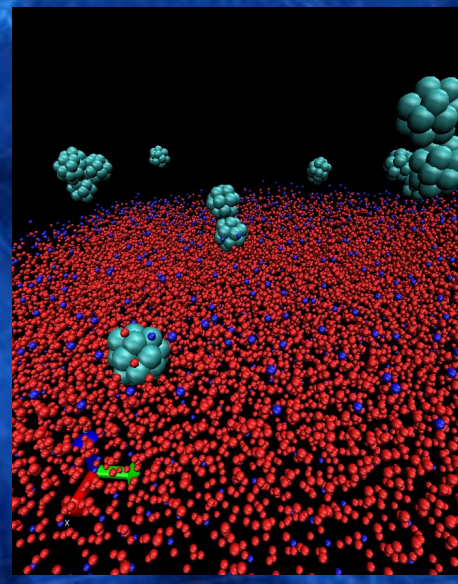
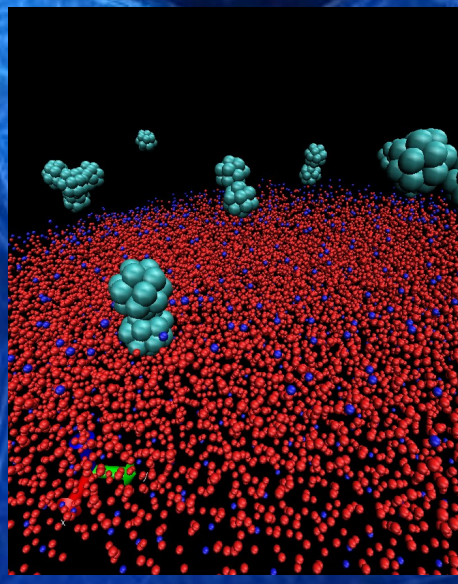
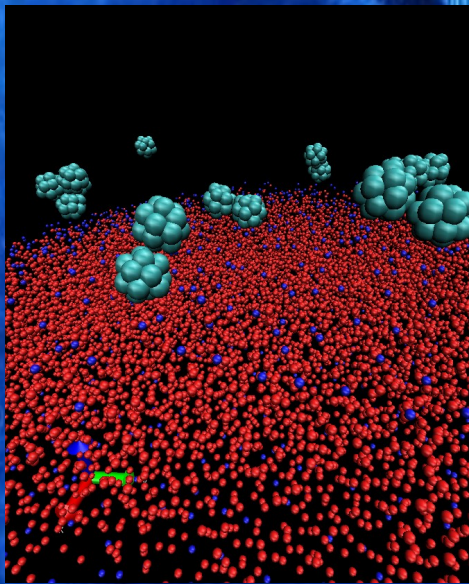
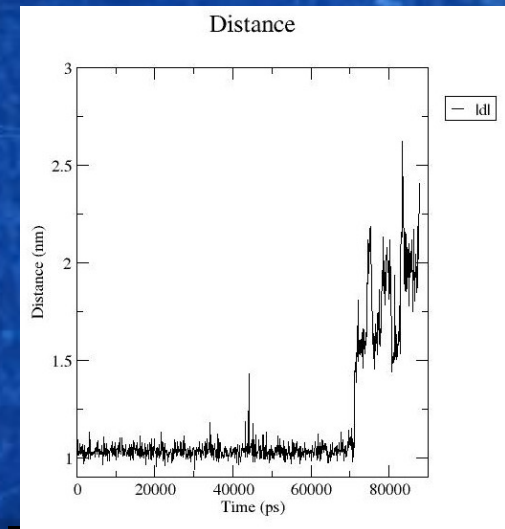
- Membranes & Fullerenes
- 88.000 ps simulation



(1) and (2) Images from: Molecular Dynamics – R.U.G. (2008)
Data obtained from: “Computer simulation study of fullerene translocation through lipid membranes” by Jirasak Wong-Ekkabut, Svetlana Baoukina, Wannapong Triampo, I-Ming Tang, D. Peter Tieleman and Luca Monticelli

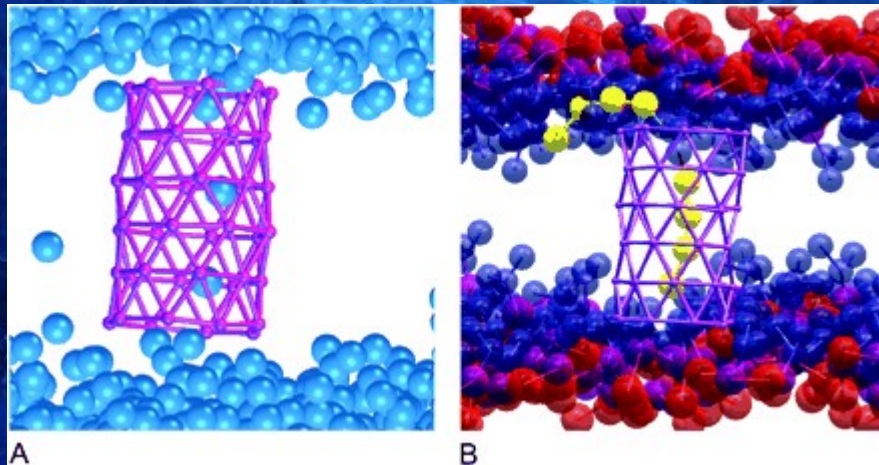
Detail simulation

- Aggregates in water
- Disaggregate after entering

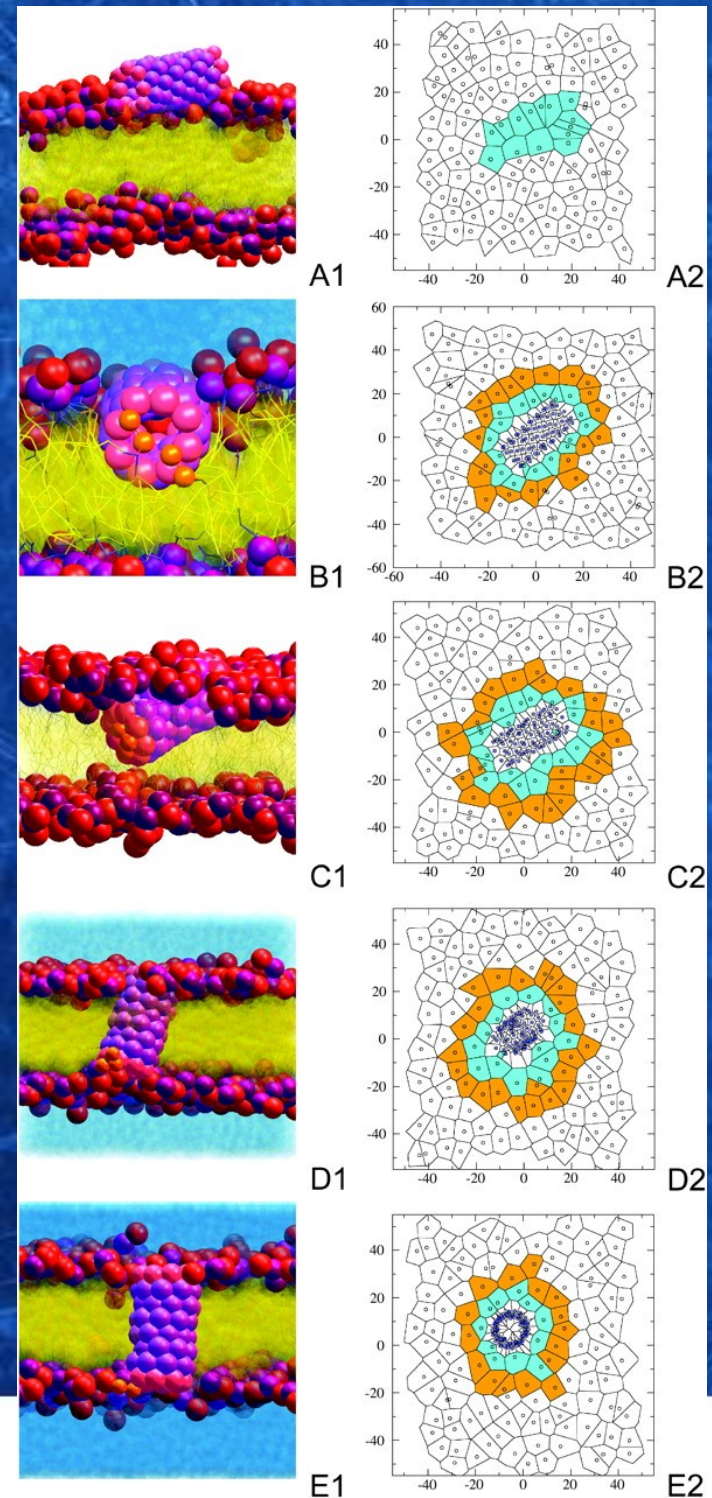


Simulations

- Insertion of a nanotube inside a membrane
- Hydrophilic caps



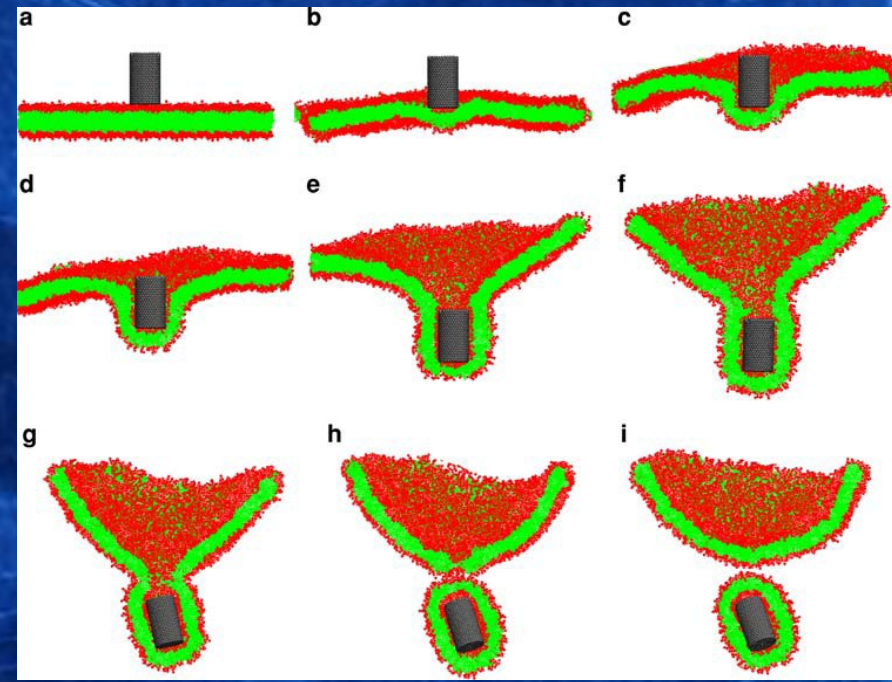
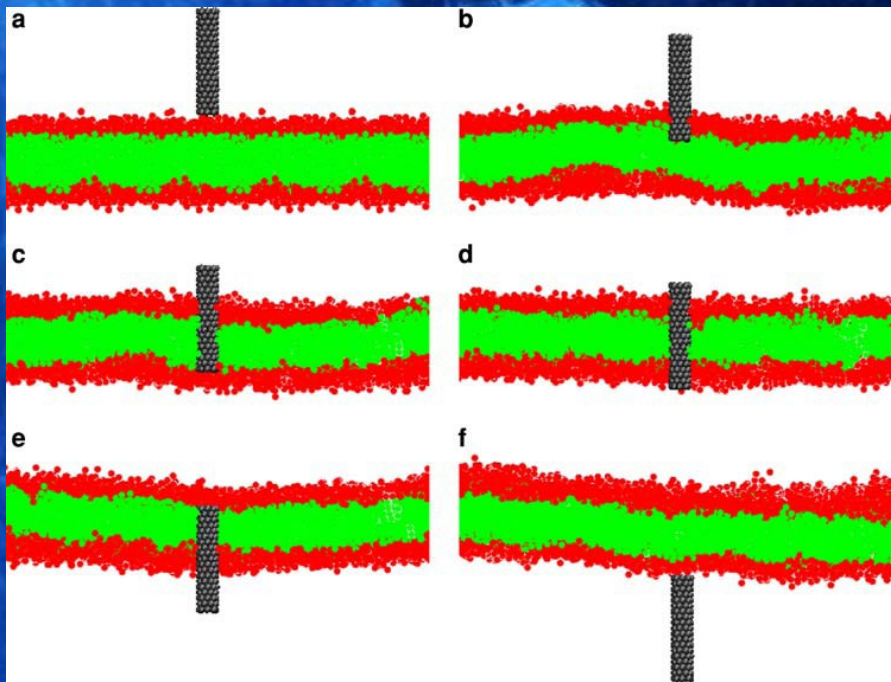
(1) and (2) Images from: Dept Chemistry – University of Pennsylvania, Philadelphia (2005)



Simulation nanotubes

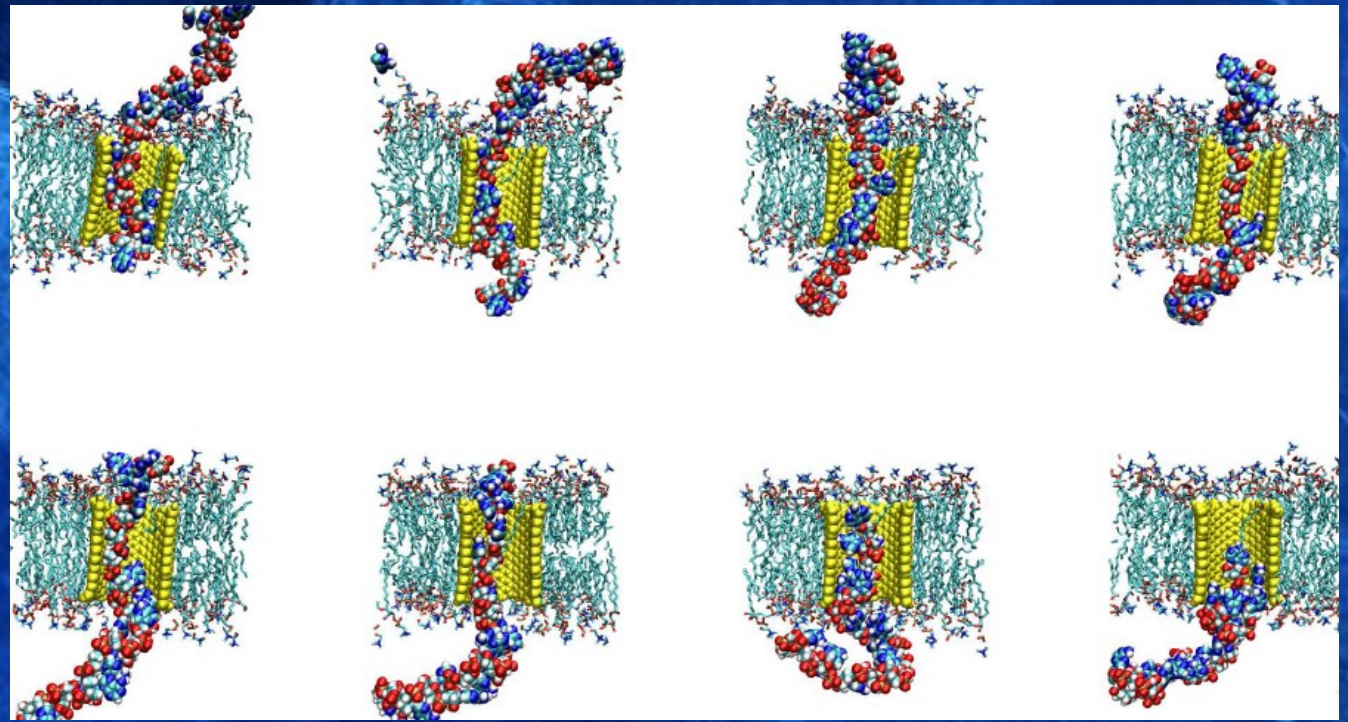
- Coarse grained
- SWNT

MWNT



Simulation RNA through a nanotube

- Potential gradient
- Threshold

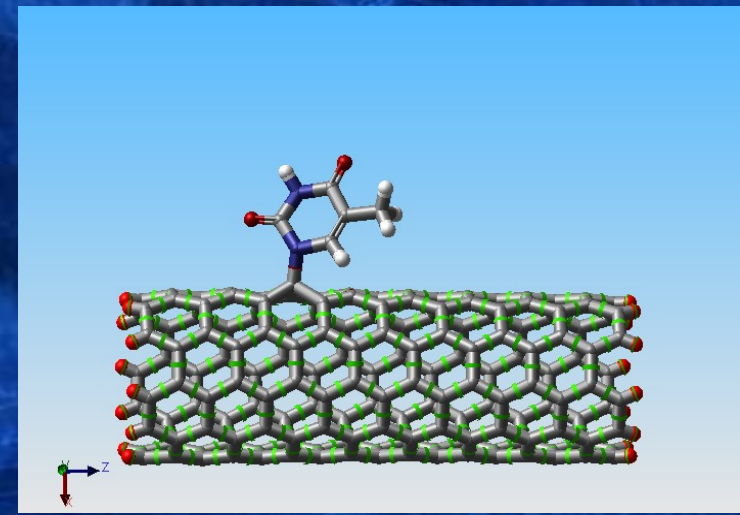
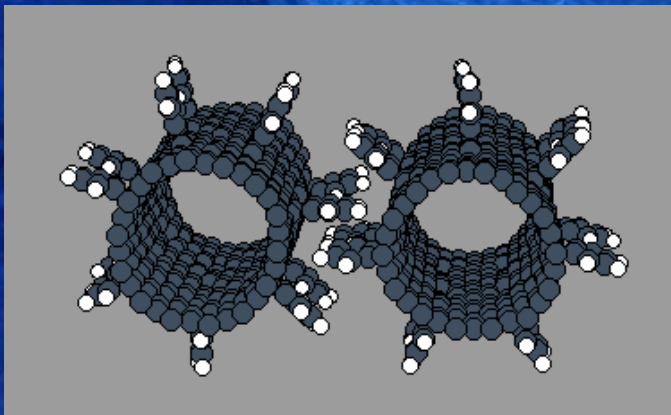


Conclusions

- Coarse-grained simulation for nanotubes
- Simulation needed to design at nano scale
- Increasingly larger systems
- Nanotubes will be used more and more
- The affinity of nanotubes for membranes

Future perspectives

- Longer (or bigger) simulations
- Nano technology used more and more
- New medical applications
 - Drug targeting / delivery



Thanks to:

- The Molecular Dynamics Group
 - Prof. S.J. Marrink
- GBB institute
- Faculty of Mathematics and Natural Sciences

Questions ?



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Molecular & Mesoscopic Dynamics in Complex Systems

Literature

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• S.J. Marrink, A.H. de Vries, A.E. Mark. Coarse grained model for semi-quantitative lipid simulations.

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Fullerenes & Martini lipids

