A Closer Look at Molecular Interactions on the Nanoscale

With the prospective work presented here we introduce possible applications for Molecular Dynamics simulation (MD) to nanotechnologists. We provide our biological, physical, and chemical background with the bottom-up concept of MD to build systems up to several 100 nanometers. With MD, dynamic processes of molecular interactions can be observed at any moment like a traffic jam from the supervision helicopter.

Dr. Lukas D. Schuler, Dr. Christian D. Berweger

Advantages

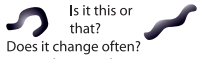
make the invisible visible
validate concepts
make the unlikely happen
study extreme conditions

Benefits

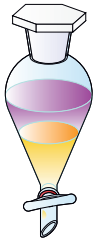
avoid dispensable synthesis
definitely explain effects
outsourcing to specialists
coaching by MD experts

Observe…

solvated structures



Is it this or that?
Does it change often?
Does it keep its shape?
How long?

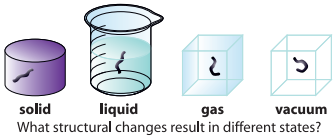


In which solvent does it dissolve?
Do solvents mix in an interphase?

Does it stay here
or inbetween
or there?

Do they exchange?
How fast?

… structures in aggregation states

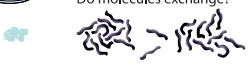


What structural changes result in different states?

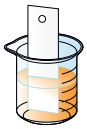
What happens under extreme conditions such as high pressure at low temperature?

Do we get aggregates or solutes?

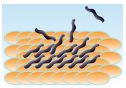
Does it form insoluble aggregates?
Do molecules exchange?



… atomic sorption or adherence in detail

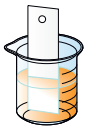


Do molecules fit into place?

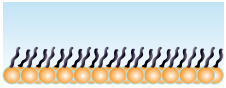


Do they form a firm surface coating?

Do molecules attach strongly?
Do structures force them into a preferred orientation or shape?



What are the forces and dynamics between surface molecules?



What surface tension does result in a nano-droplet?

… diffusion in complex materials

What time dependence on the liquid properties, e.g. their viscosity, do we obtain in simulation?

How do small molecules travel through porous materials like polymers or gels? Are they absorbed?

What is the influence of charged particles or electrical fields on the diffusion?

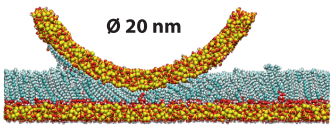
All these simulations can be done …

- in comparison to experiments and for validation
- observing every single move of every single atom
- in narrow spaces inaccessible to experiments
- without marker molecules
- without measurement devices (it's calculation).

Close-up

with MD Simulation

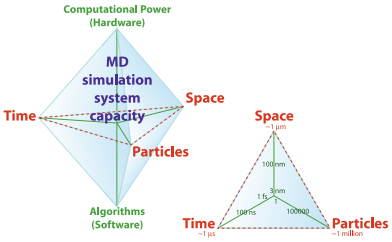
Nanotip indentation of a coated surface



A 10 nm radius silica tip makes contact with a silica substrate, coated with a self-assembled monolayer of alkyl silanes for a study of friction and wear. The snapshots shows deformation and damage to the coating layer due to the tip.

Nanotribology of Anti-Friction Coatings in MEMS
M. Chandross, C. D. Lorenz, G. S. Grest, M. J. Stevens, and E. B. Webb III
Journal of Minerals, Metals, and Materials (JOM), 57, 55 (2005).

Growing Capacity in MD Simulations

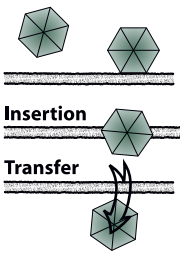


Molecular Dynamics simulation system capacity is limited only by computational power and efficient calculation algorithms.
The demand of simulated time, space and particles is interconnected in a magical triangle that has a fixed format, limited by the height of the bipyramid.
The system limits of the magic triangle are growing every year in nanometers, nanoseconds and several hundred thousand of particles. Faster CPUs, parallelization, more memory and grid computing lead to simulate microseconds, micrometers and millions of particles at atomic details.

Prospective MD Studies

Does a nanoparticle transfer through a cell membrane?

Adsorption/Adhesion



Dynamics can be virtually initiated upon request and the energies involved can be studied in detail.

We sketch a concept for nanoparticle assessment in a biophysical environment by Molecular Dynamics simulation as a prescreening test to assist expensive toxicological surveys.

A cell membrane should be recognised as a liquid crystal and elastic-porous material.

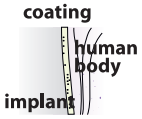
Computer simulation study of fullerene translocation through lipid membranes. J. Wong-Ekkabut, S. Baoukina, W. Triampo, I. Tang, F. D. Tieleman, L. Monticelli, University of Calgary Nat Nanotechnol. 2008 Jun; 3 (6):363-8

Optimise the properties of an implant coating

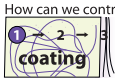
Clinical trials or animal experiments are costly and tightly regulated and shall be reduced to the minimum necessary.

implant surgery

A clinical vision is to control the immuno-response of the human body until inflammation is over by an optimal drug elution from the implants interface.



How can we control the rate of drug release?



1. drug release from containment
2. drug diffusion through coating
3. drug release into body compartment

The physical properties of independent barriers can be simulated and studied in detail to find controls of release rates.

Knowledge Based Suggestion, Conclusions

The MD method[1] has been established by academic groups over decades, but is not easily adopted to satisfactory degree by newcomers. It works at the scale experimentalists are applying Atomic Force Microscopes and other analysis and manipulation tools. Its time-scale runs from femtoseconds up to several 100 nanoseconds. Sometimes, experiments succeed well, and yet they are not completely understood. Observing molecular interactions is a key to understand the influence of underlying physical interactions on the performance of chemical composition. It can help avoid dispensable synthesis by assessment of derivatives or different conditions like pressure, temperature or concentration by computer simulation. On the other hand experimental measurements can be validated.[2]
It is possible to investigate probes in narrow spaces where any measurement method would introduce disturbance. Adhesion or aggregation are dynamic processes and can only be understood by dynamic observations at high resolution in time. For situations in which measurements cannot clarify the picture, such as structural dynamics in liquids, diffusion within nanopores, or preferred sorption configurations at surfaces, MD is a means to satisfy this observatory and conclusive need. In theory, the applicability of MD is only limited by the number of particles, hence the computational power and memory usage and the restrictions and fail-safeness of the methods used. In practice, applying MD without expertise will fail.
We suggest experimentalists to partner with simulation experts. Simulation experts offer to work hand-in-hand with experimentalists to improve know-how in R&D and quicker solve design issues. They are able to consult researchers for the choice of new and upcoming simulation methods and solve their questions by complementary approaches, or they can coach them at their needs to learn the theoretical methods.

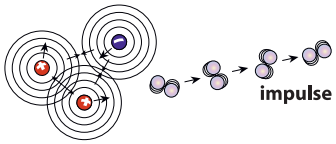
[1] L. Schuler, Simulation News Europe 2008, in press
[2] L. D. Schuler, X. Daura and W. F. van Gunsteren, J. Comput. Chem. 2001, 22, 1205-1218

MD Method

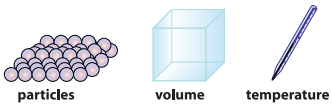
build molecules

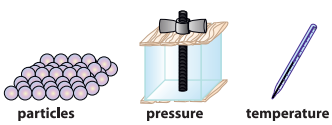
apply physics and chemistry

potential energy kinetic energy



choose thermodynamic constraints





The chemical properties are described by empirical potentials for all atoms included. Physical laws are enforced such as Newtons equations of motion, energy conservation, velocity distribution for a given temperature. The dynamics are integrated by applying small time steps in the range of 10^{-15}s.

xirrus simulation

xirrus GmbH, Buchzelgstr. 36, 8053 Zürich, Switzerland · www.xirrus.ch · info@xirrus.ch · +41 44 741 01 74

xirrus GmbH is a reliable technology partner for Molecular Dynamics (MD) simulation, which can provide you the following services:

- Support your R&D with detailed insight into nanoscale spaces by bottom-up computer simulations.
- Help you avoid dispensible synthesis by evaluating important molecular interactions before lab work.
- Quick interpretation of simulation models and results by our experts.
- Hand–in–hand development of systems with your experimentalists.
- Support you with new methods and coaching at your demand.
- Control risk of failure by outsourcing of complex simulations.

Dr. Christian D. Berweger and Dr. Lukas Schuler promoted in MD and are experienced in implementation, software development, analysis and quality ensurance of modelling and simulation for nano-scale and other particle or agent based systems. They are members of the Arbeitsgemeinschaft Simulation (ASIM).

2001 foundation of xirrus GmbH
2005 development of «ximulon» for simulation services
2006 process management for finance consultancy of high risk assets
2007 Simulationen zur Verbesserung des FLARM-Funkprotokolls
C. D. Berweger, L. Schuler, segelfliegen 3 (2008) 30-33