A Closer Look at Molecular Interactions on the Nanoscale

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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 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 interface?
  - Do they stay there or hibiscus there?
  - Do they exchange? How fast?

**structures in aggregation states**
- solid
- liquid
- gas
- vacuum
- 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 form into a preferred orientation or shape?
- What are the forces and dynamics between surface micelles?

**... diffusion in complex materials**
- What time dependence on the liquid properties, e.g. 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 matter molecules
- without measurement devices (it’s calculation).

**Close-up with MD Simulation**
- Nanotip indentation of a coated surface
  - 80 nm

**Prospective MD Studies**

**Does a nanoparticle transfer through a cell membrane?**

**Optimise the properties of an implant coating**

**Knowledge Based Suggestion, Conclusions**

**xirrus simulation**

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 dispensable synthesis by evaluating important molecular interactions before lab work.
- Quick interpretation of simulation results 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.

**MD Method**
- build molecules
- apply physics and chemistry
- repulsion
- attraction
- potential energy
- kinetic energy
- choose thermodynamic constraints

**The MD method** has been established by academic groups over decades, but not widely adopted in industry. The goal is to base software and models on applying these methods to real-world problems. The main advantage of MD is its ability to provide detailed information on the atomic-scale interactions of a system. MD simulations can be used to study the behavior of biological molecules, the properties of materials, and the dynamics of complex systems. The results of MD simulations can be used to predict and optimize the performance of new materials and drugs.

**References**

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