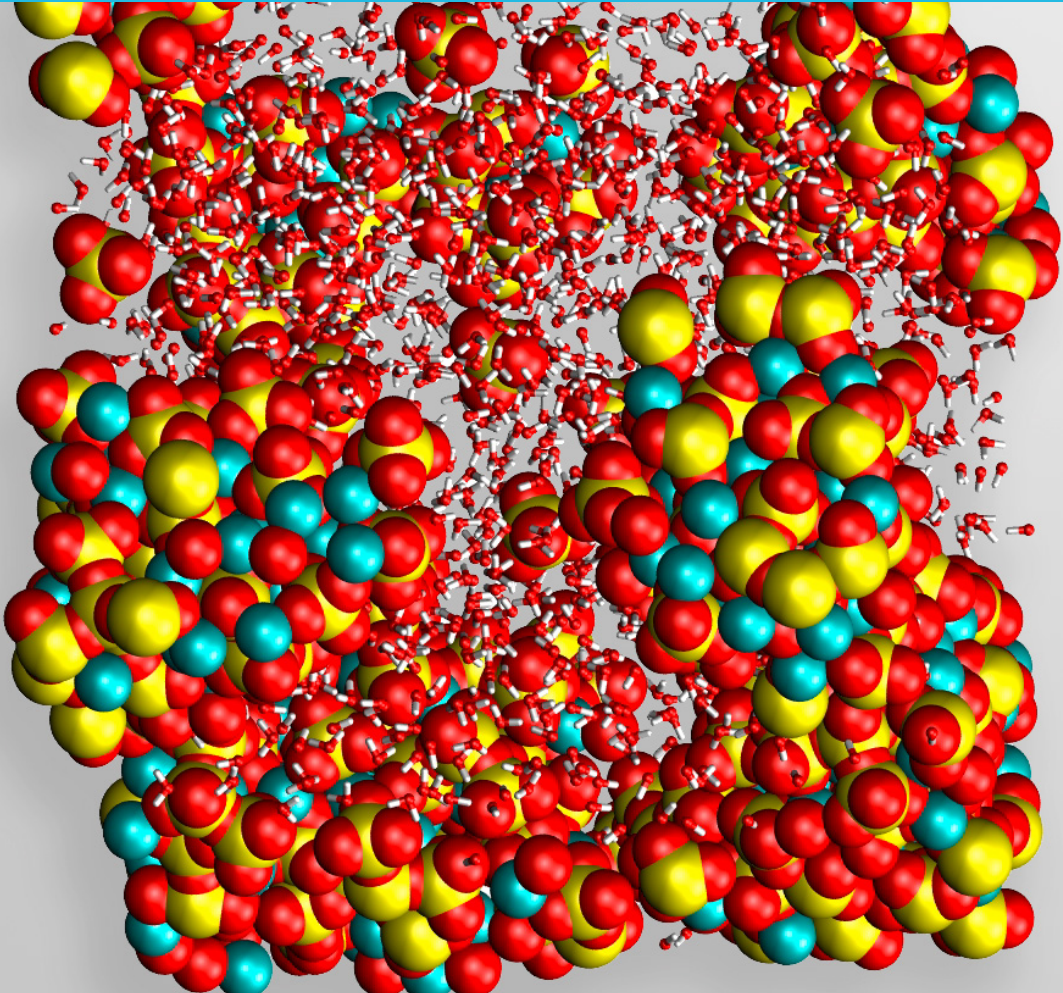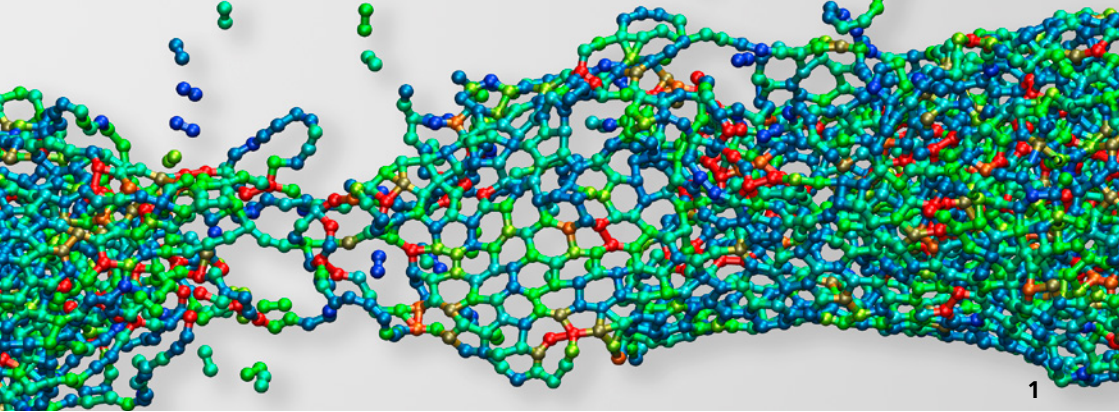**Fraunhofer**

SCAI

VIRTUAL MATERIAL DESIGN

VIRTUAL MATERIAL DESIGN

Many of the challenges of the 21st century – such as the development of new and improved energy systems, environmentally-friendly systems, and improved ICT technologies for health and mobility – will rely on the availability of a new generation of materials. That those materials can be designed and created depends on interdisciplinary research teams from science and application-oriented engineering producing new technologies in the areas of nanotechnology and material science.

Applied research and development at the department of »Virtual Material Design « (VMD) is focused on multiscale modeling and numerical simulation in material science and nanotechnology. Massively parallel computers are employed to simulate new materials at the nano-, micro- and macro-scale using modern multiscale methods in quantum mechanics, molecular dynamics and continuum mechanics. The aim is to use the (computational) »virtual laboratory« to create and to study new innovative materials with specific, targeted properties in order to propose their structure and design before they are synthesized in reality. This approach to material design promises to avoid many expensive prototypes and experiments (in real world laboratories). Hence, the costs of development can be substantially reduced with the help of numerical simulation. In addition, completely novel materials can be found. In this framework, a central topic besides multiscale modeling is the development and implementation of efficient parallel software packages for material science and nanotechnology simulation.

Quantum mechanics	Molecular mechanics	Continuum mechanics
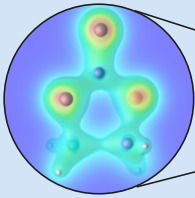
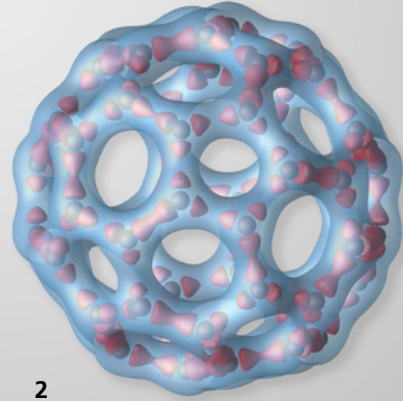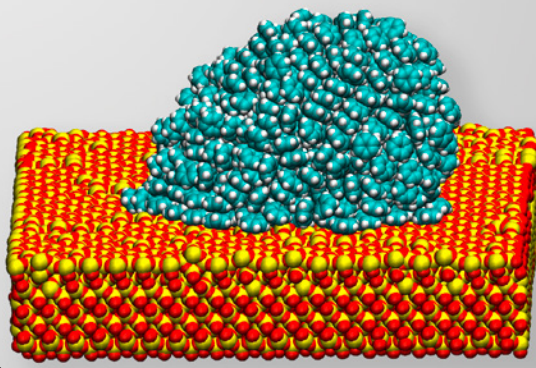| Chemical structure of an electrolyte	Diffusion / chemical potential in an electrolyte	Ion migration in an electrolyte
1 A – 1 nm	1 nm – 100 nm	1 mm – 1 m

2

NANOSCALE AND MULTISCALE VIEW

Nanostructured materials exhibit different material properties than their bulk counterparts, since their high surface to volume ratio results in more surface exposure to nanoparticles and thus leads to highly reactive materials. Many new materials are created solely by redesigning the surface structure of existing materials, enhancing such properties as impermeability, heat resistance or anti-bacterial properties. Nevertheless, nanoparticles and special nanostructures are also applied to design new innovative materials which, among others, include meta-materials and nano-composite materials.
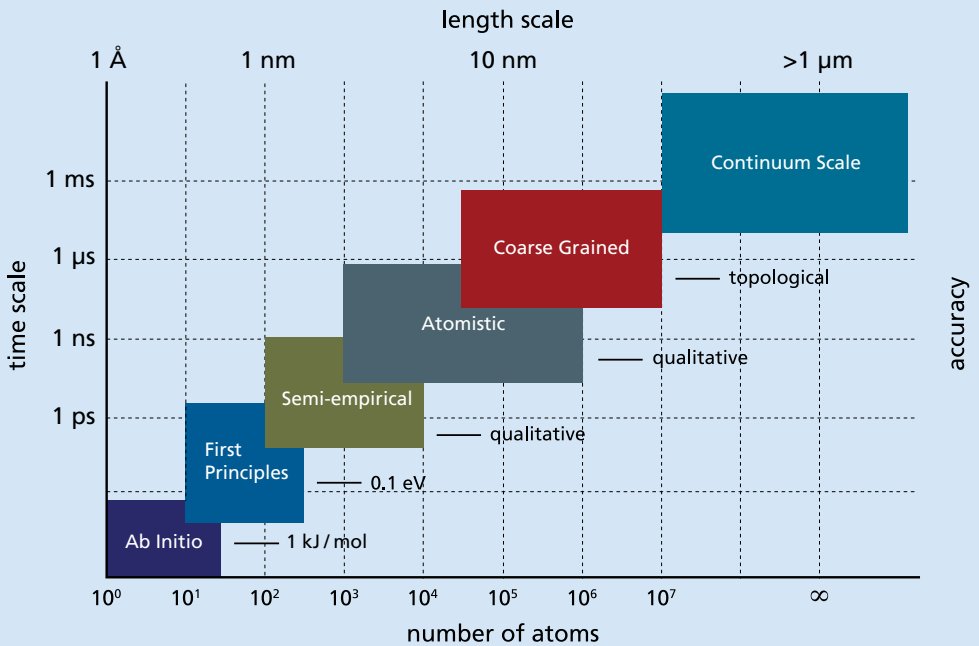
The resulting effective macroscopic properties are mostly a consequence of the detailed structure at the nano and micro scale. Since at the scale of molecules, atoms and electrons, all physical systems are in principle described by quantum mechanics, the underlying mathematical model is the Schrödinger equation. However, to simulate one second of behaviour of one millilitre of material at the atomic scale, the calculation would take approximately 10^{20} years computing time, even on today's largest supercomputers (cf. the lifetime of sun is about 10^{10} years). Therefore, it is necessary to adopt a multiscale view to take into account that physical effects occur at many scales in space and time. Hence, mathematical models and numerical simulations must consider the respective scales at which behaviour is influenced. In particular, the up-scaling of models has to be done carefully since quantum effects and microscopic effects have consequences on the macroscopic level.

1

2

LEVELS OF MATHEMATICAL MODELS

length scale

| 1 Å | 1 nm | 10 nm | >1 μm |

time scale

accuracy

1 ms

1 μs

1 ns

1 ps

Continuum Scale

Coarse Grained

topological

Atomistic

qualitative

Semi-empirical

qualitative

First Principles

0.1 eV

Ab Initio

1 kJ / mol

number of atoms

10^0 10^1 10^2 10^3 10^4 10^5 10^6 10^7 ∞

■ **Ab Initio Methods:** e.g. Quantum Monte Carlo, Coupled Cluster
■ **First Principles Methods:** e.g. Density Functional Theory
■ **Semi-empirical Methods:** e.g. Tight Binding
■ **Atomistic Methods:** e.g. Force Field Molecular Dynamics
■ **Coarse Grained Methods:** e.g. Coarse Grained Molecular Dynamics
■ **Continuum Scale Methods:** e.g. Continuum Mechanics, Computational Fluid Dynamics

3
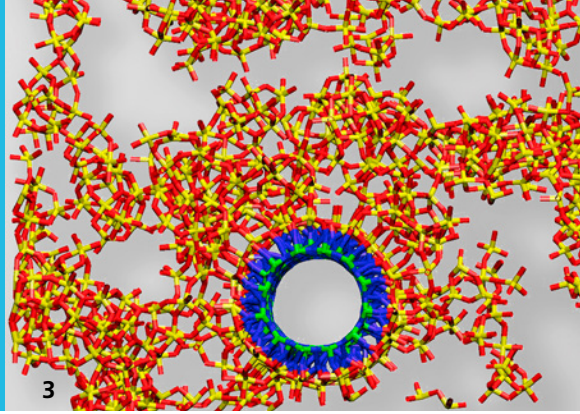
OFFERS

Fraunhofer SCAI offers individual solutions to our partners and customers in the following areas:

• Multiscale modeling and numerical simulation for material science and nanotechnology.
• High performance computing in quantum mechanics, molecular dynamics and continuum mechanics.

In particular this includes mathematical modeling and development of algorithms as well as customized software and numerical simulation.

PRODUCTS

An essential basis for designing novel materials is the understanding of their properties at the nanoscale. Molecular dynamics simulation is an important tool for the analysis of a material at that scale. To this end, Fraunhofer SCAI offers Tremolo-X, a massively parallel software package for numerical simulation of molecular dynamics. Here, great emphasis has been placed on the parallel implementation and its efficiency.

1 *Benzene droplet on a silicon oxide*
2 *C_{60} bucky ball with isosurface of the electron density*
3 *Reinforced nanomaterial: boron nitride nanotube in an silicon oxide matrix*

TREMOLO X

1
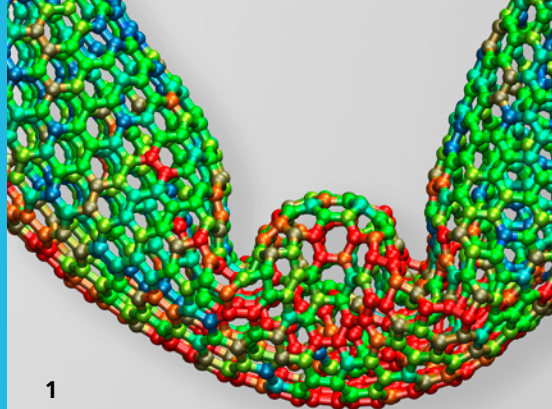
TREMOLO-X

Molecular Dynamics Simulation
Tremolo-X is an efficient software package used for the numerical simulation of interactions between atoms and molecules, the molecular dynamics. It provides an environment in which to design new innovative materials.

Parallel Efficiency
Tremolo-X uses highly efficient state-of-the-art algorithms for the treatment of short- and long-range potentials, where great emphasis has been placed on the parallel implementation and its efficiency. All potential types are included which are commonly used for the modeling of systems in the areas of material science, nanotechnology and biophysics.
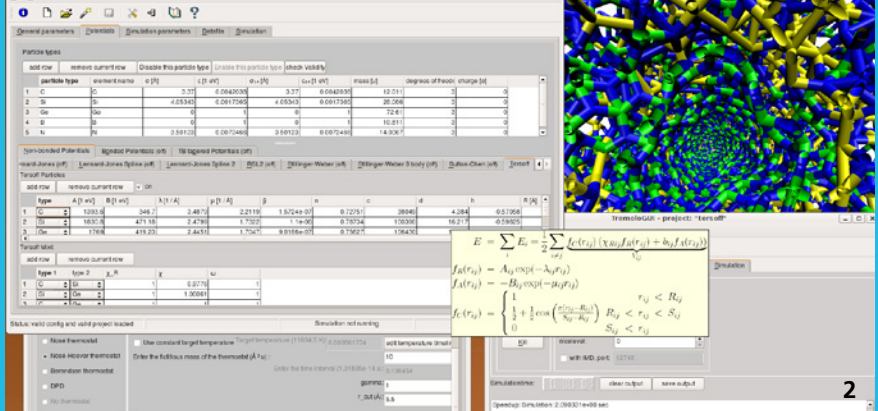
Graphical User Interface
Tremolo-X also includes Tremolo-X-GUI, which is a user-friendly graphical user interface frontend. This provides an easy set-up and analysis of numerical experiments.

Modeling
Tremolo-X has already been successfully applied in many different practical projects in different areas. The focus is on computations in nanotechnology, material science, biochemistry and biophysics.

FEATURES

- User-friendly graphical user interface
- Parallel version for distributed memory computers (MIMD) with the message passing interface (MPI)
- Parallel implementation of reactive many-body potentials of Brenner, Marian, Tersoff, Feuston-Garofalini, Stillinger-Weber and Sutton-Chen
- Parallel implementation of fixed bond, angle, torsion (dihedral) and inversion potentials
- NVE, NVT and NPT ensemble, structural optimization and dissipative particle dynamics (DPD)
- Several time integrators and local optimizers: Verlet, multistep like Beeman-Verlet as well as Fletcher-Reeves and Polak-Ribière
- Replica exchange methods like Hybrid Monte Carlo and Parallel Tempering
- Computation of many derived quantities and measures, e.g. diffusion coefficients, stress-strain diagrams, elastic constants, distribution functions, correlation functions and shortest-path-ring statistics
- Fast implementation of short-range potentials via linked-cell method and parallelization by dynamic load-balanced domain decomposition
- Fast algorithms for long-range potentials: Particle-Mesh-Ewald with domain decomposition and parallel 3D-FFT and parallel multigrid. Also Barnes-Hut/fast multiple methods and parallelization by space-filling curves
- Simply extendible to new potential types by modularity

1 *Bending of a double walled carbon nanotube*

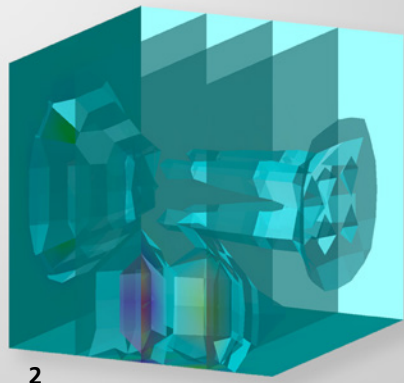**2** *Graphical user interface (GUI) of Tremolo-X*
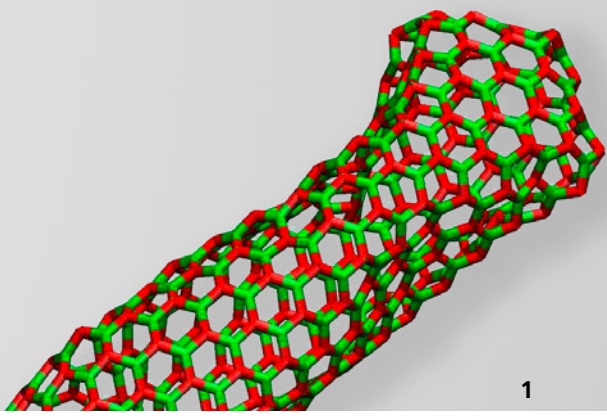
NANOMATERIALS

Nanoparticles exhibit exceptional material properties and thus provide a wide range of possible applications in various areas such as lightweight construction (composite materials, concrete), energy and environmental engineering (batteries, fuel cells, hydrogen storage), electronics (cooling, transistors, field emission display), medicine (sensor technology, drug-delivery) and also information and communication technology.

For example, carbon nanotubes (CNTs) show outstanding mechanical, thermal and electrical properties. Hence, they are already used in industrial applications for mechanical reinforcement and optimization of electrical conductivity of polymer composite materials. Besides carbon or boron-nitride based nanoparticles (Fullerene, CNTs, graphene, BN-NTs) also ceramic and metallic nanoparticles have been synthesized with remarkable properties.

In the context of design and production of nanomaterials many ques-tions and challenges emerge. To this end, the VMD department provides several efficient software tools to tackle these problems.

**1** *A capped boron nitride (BN-NT) nanotube*

SIMULATION OF ION MIGRATION

The combined diffusion and convection of ions through different materials is the foundation of a variety of technically interesting processes, ranging from battery operation via concrete degradation to the use of biomembranes. NPNP (Nonlinear Poisson Nernst Planck) is a software package for numerical simulation of complex ion migration processes of multiple ion species while observing the coupling of an electric field and charges in arbitrary geometries. NPNP is designed for time-dependent problems.

Features
• Multiple ionic species can be handled by NPNP.
• To compute time dependent solutions, stabilizing iteration procedures are used.
• Complex geometries are treated with adaptive meshes (2D and 3D available).
• The tool is optimized for the use with multiprocessor machines and shared memory. In the future this will be extended to distributed memory machines.
• The construction of the NPNP-software allows use to be made of results from prior atomistic simulations (e.g. from Tremolo-X).

**2** *A concentration profile of a perturbed electrolyte.*
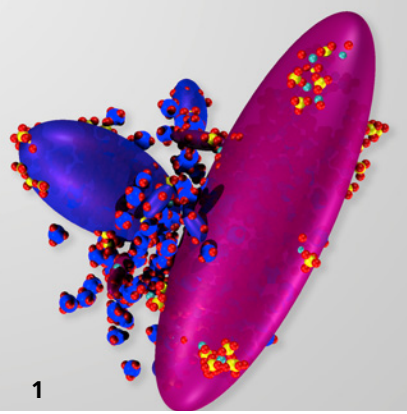
INNOVATIVE CEMENTITIOUS MATERIALS

Cement and cementitious materials are of paramount importance in today´s society. In light of their widespread use in the construction of bridges, airports, residential and office buildings and countless other key components of modern infrastructure their stability and reliability is of incomparable significance.

However, it is well known that the leeching of ions has a destabilizing effect on those materials, a process which is accelerated by industrial pollution and acidic rain – everyday occurrences in urban centres. With this background in mind, it may come as a surprise that many fundamental questions relating to cement and cementitious materials have not yet been answered by science.

One such open issue is that there is no reliable knowledge about the nanostructure, the basic building block of cementitious materials. Furthermore, there is still a lack of models describing the progression of ion leeching from the cement matrices. The VMD department supplies tools, which solve these open problems.

1 *A coarse grained model of a cementitouis C-S-H gel*

2
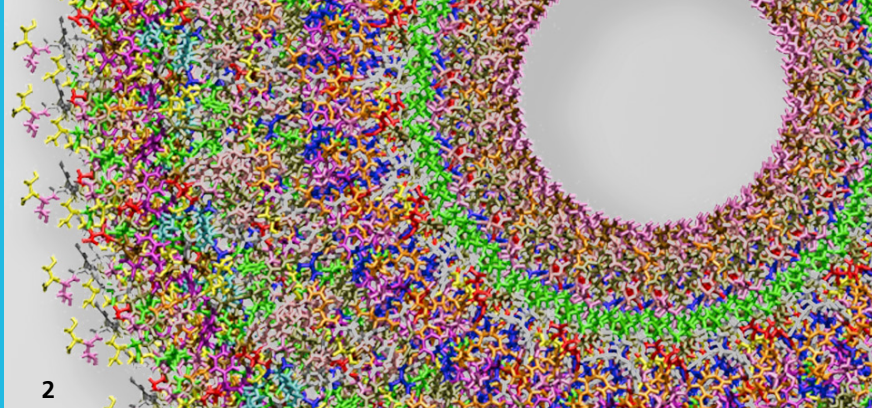
HIGH PERFORMANCE COMPUTING

Numerical simulations in quantum mechanics, molecular dynamics and continuum mechanics are highly demanding in terms of computational requirements. To this end, the research in the VMD department also focuses on the development and implementation of state-of-the-art highly efficient and parallel scalable simulation tools for high performance computing clusters.

2 An atomistic model of the tobacco mosaic virus

CUDA RESEARCH CENTER

Because of their leading research in numerical simulation using parallel computing, Fraunhofer SCAI and the Institute for Numerical Simulation at the University of Bonn have officially become one of the first German NVIDIA CUDA Research Centers. One focal point is R & D regarding the parallelization of existing simulation codes to run on machines with multiple graphics processing units (GPUs). The second focal point is the development of massively paralleled multi-GPU based software packages for numerical simulation in the natural and engineering sciences. In the VMD department the goal is to develop a massively parallel, completely multi-GPU based high performance molecular dynamics software package. To this end, the SCAI software Tremolo-X is adapted. SCAI's customers from industry and research institutes will profit from the transfer of knowledge from basic research to practical applications.

CONTACT

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Front cover: Cementitious
C-S-H gel at the nanoscale