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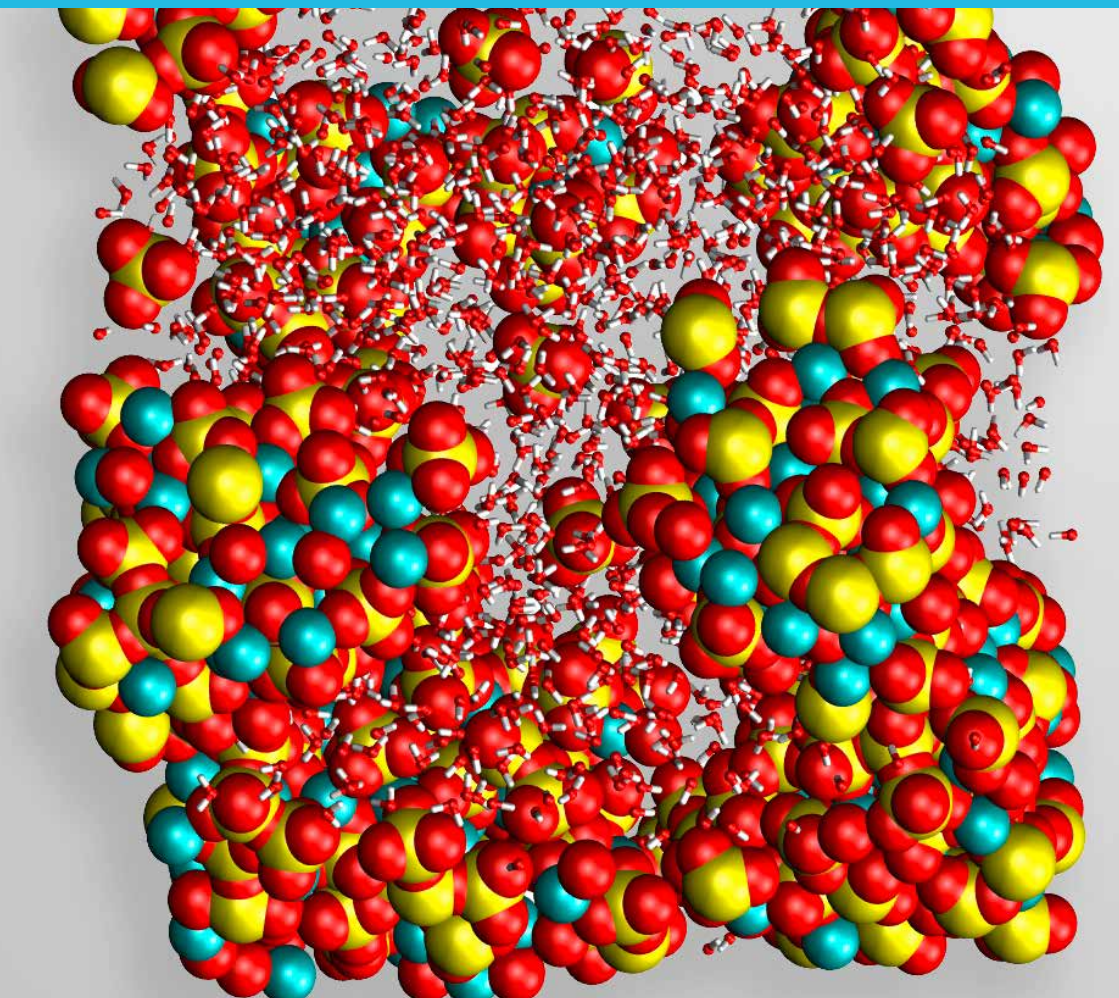
FRAUNHOFER INSTITUTE FOR ALGORITHMS
AND SCIENTIFIC COMPUTING SCAI

VIRTUAL MATERIAL DESIGN



1

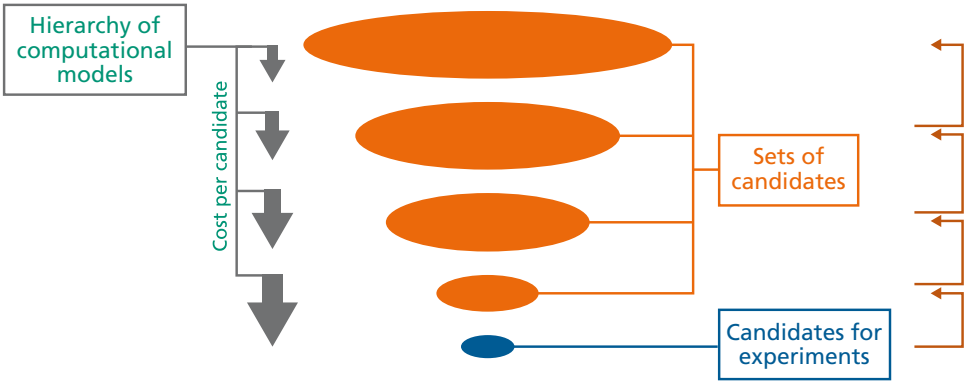
VIRTUAL MATERIAL DESIGN

1 *Isopotential surfaces of valence electronic density in gallium arsenide.*

New technology is largely driven by innovative materials with specific desired properties. Hence, materials science, chemistry and nanotechnology are key technologies of our century. These interdisciplinary fields incorporate fundamental natural sciences, application-oriented engineering technology and also applied mathematics, computational science and data science.

Applied research and development at the Department of Virtual Material Design (VMD) is focused on modern multiscale modeling and efficient numerical simulation techniques in computational materials, science and chemistry. VMD uses state-of-the-art numerical methods for high dimensional problems, optimization, machine learning and data analysis. In particular, SCAI combines these technologies with in-house knowledge and empirical data in a sophisticated manner, leading to a virtual material design approach.

The overall aim is to optimize, to create and to study new and innovative materials and molecules in the virtual computer lab in order to assist the practical development process by substantially reducing its cost in time and money. In this framework, the development and implementation of efficient software tools for materials science and nanotechnology is also a central topic.



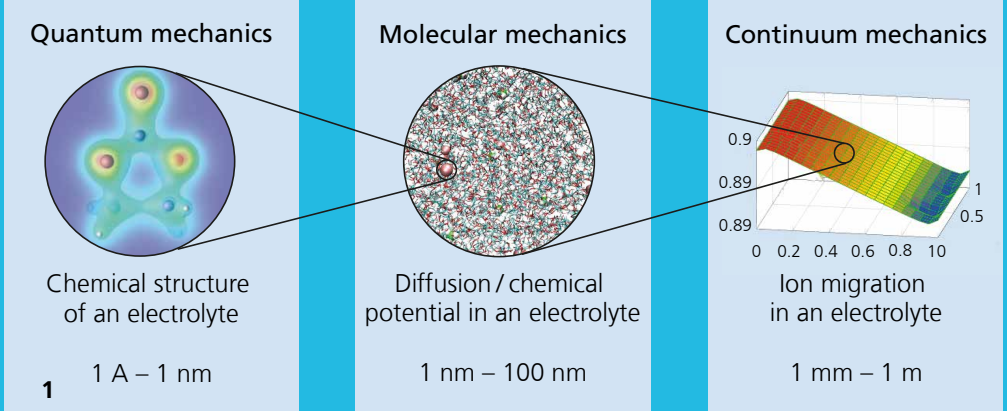
INNOVATIVE DATA-DRIVEN DESIGN

2 *High throughput virtual screening approach; reentry at any stage for refinement is possible.*

Empiricism (e.g. experiments) and model-based theory (e.g. quantum mechanics) are the two dominant scientific paradigms. Over the last few decades, computational science has been successfully established as a third paradigm. Recently, the availability of experimental and simulation data has resulted in the emergence of so-called data-driven approaches as an additional, fourth paradigm of science.

VMD follows the idea of data-driven approaches by combining existing knowledge, empirical and simulation data together with data analysis, machine learning, statistical methods, high-dimensional optimization and multiscale modeling techniques to develop and optimize new materials and processes. In this context, VMD performs research and development on machine learning and data-analysis approaches for computational materials science and chemistry and follows a *gray-box* modeling ansatz, which unifies in some sense all paradigms.

The aim of *white-box* models is an exact physical description of the modeled system (by, e.g. PDEs), while the purpose of a *black-box* model is to reproduce the input-output behavior of a system (by, e.g. deep learning neural networks). However, in many cases, establishing white-box models is too complex and the amount and quality of data for black-box models is often insufficient. Hence, approaches which are based on a mixture of black-box and white-box models, i.e. gray-box models, are in general a promising powerful tool.



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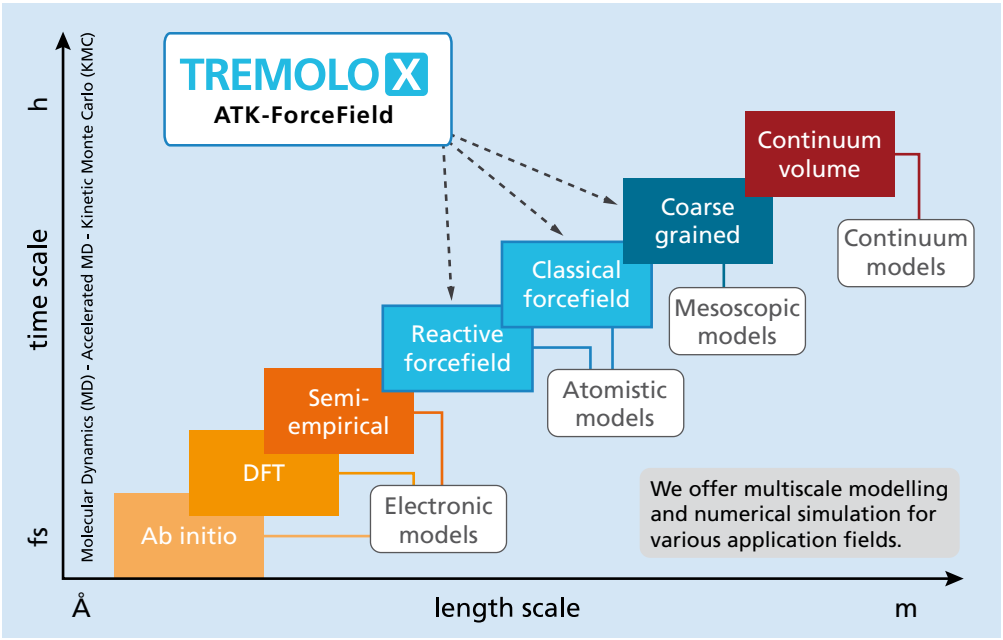
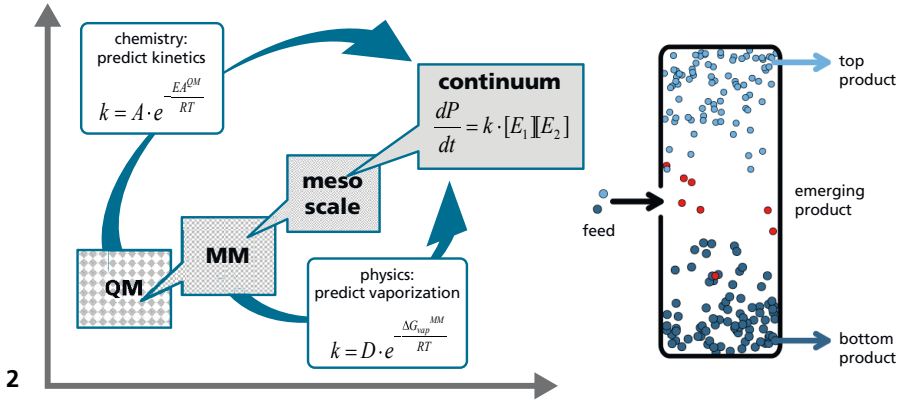
MULTISCALE MODELING

1 *Multiscale model of an electrolyte in Li-ion batteries.*

An essential basis for designing novel materials and molecules is the understanding of their properties on the nanoscale and their effect on the macroscale. Hence, in most cases multiscale models in space and time (which are in particular based on the atomistic level) are necessary to describe a material accurately and to predict its long-term behavior.





NUMERICAL SIMULATION

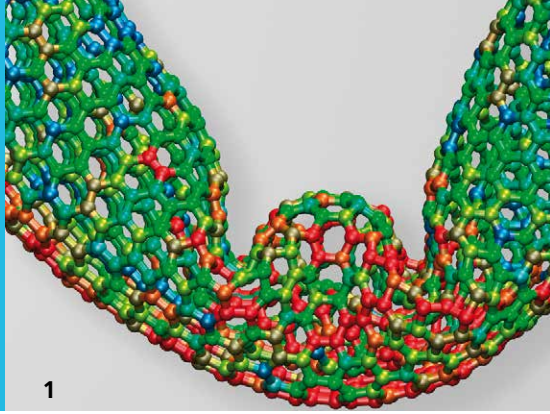
2 *Integrating chemical, physical and continuum aspects, e.g. for reactive distillations.*

Using models and tools from computational materials science and computational chemistry, a wide range of properties can be predicted with high accuracy. These tools allow the simulation and study of various processes:

- Electronic and magnetic properties
- Mechanical properties
- Electrochemical properties
- Chemical properties
- Thermodynamical properties
- Reaction pathways
- Diffusion and migration processes
- Membrane permeability and toxicity
- Growth and processing of materials

There are many applications in various areas of the chemical and materials industry, such as semi-conductors, electronic devices, nanomaterials, ionic liquids, cementicious materials, battery materials, fuel cells, polymers, alloys, and composite materials.

TREMOLO X



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TREMOLO-X

www.tremolo-x.com

Tremolo-X provides a basis for a computational environment for the design of innovative materials, and optimization of processes.

Molecular Dynamics Simulation

Tremolo-X is a powerful software package used for the numerical simulation of interactions between atoms and molecules (molecular dynamics). It uses highly efficient state-of-the-art algorithms for the treatment of short- and long-range potentials. A wide range of potential types and parameter sets are included, which can be used for modeling of diverse systems.

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

Tremolo-X is distributed by

scapos AG

Schloss Birlinghoven 1

53757 Sankt Augustin,

Germany

Phone +49 2241 14-4400

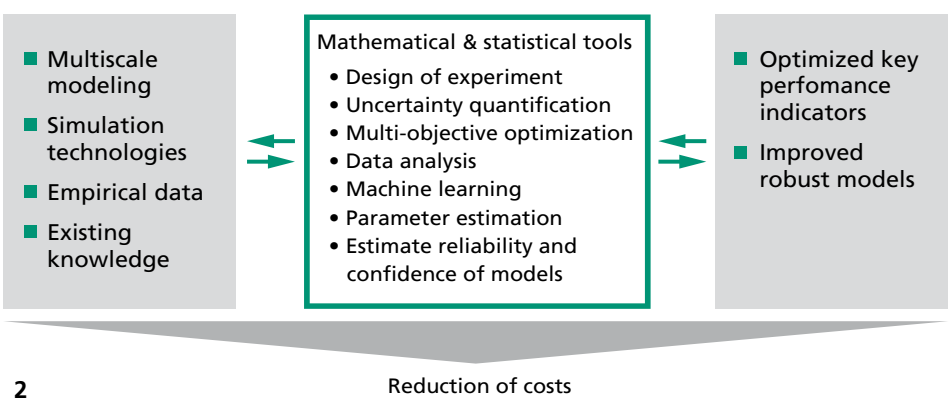
info@scapos.com

www.scapos.com

ATK-ForceField

A special version of Tremolo-X forms the numerical engine of the ATK-ForceField module, developed in partnership with QuantumWise, for their Software QuantumATK. It can in particular be used directly together with DFT and semi-empirical methods. Currently, we are extending its functionality to be easily usable within a chemo- and materials informatics context.

Quantum Wise



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SCOPE OF SERVICES

We have strong expertise in:

- Multiscale modeling, numerical simulation and data-science in materials science and chemistry
- Mathematical and statistical methods for design of experiment, uncertainty quantification, sensitivity analysis and parameter estimation
- Numerical methods for high dimensional problems and multi-objective optimization
- High performance computing in quantum mechanics, molecular dynamics and continuum mechanics
- Machine learning, surrogate models and (big) data analysis

Based on this expertise, we offer individual solutions to our partners and customers in the following areas:

- Computer-aided materials and molecular design and development
- Process optimization and efficient exploration of the design spaces
- Materials and chemoinformatics
- Integrated computational materials engineering (ICME)
- Improvement of computational models and estimation of reliability and confidence
- Simulation based decision support systems

We also offer mathematical and gray-box modeling as well as the development of algorithms and customized software tools.

1 *Bending of a double-walled carbon nanotube.*

2 *Virtual materials design approach, efficiently reducing production costs.*

CONTACT

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