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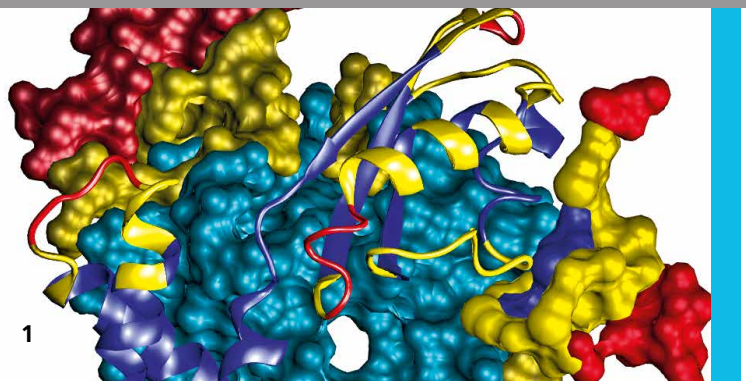

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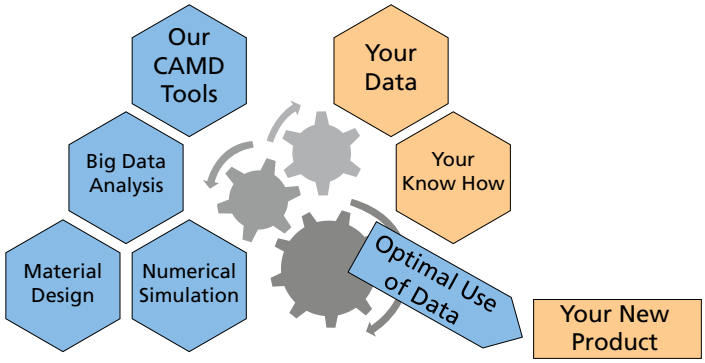

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1 *Bacterial ribosome with a bound thiostrepton antibiotic. Simulation to study the binding dynamics of the complex. The colors represent how much atomic fluctuation occurs during the simulation.*

2 *Our service at a glance.*

COMPUTER-AIDED MOLECULAR DESIGN

The Virtual Material Design (VMD) Group performs contract research and solves problems for the industry with state-of-the-art **computer-aided molecular design** (CAMD). Our aim is to support the industry in developing products and processes.

Our customers benefit from

- less expensive experiments
- shortening of development time
- saving of R+D investments

Our multidisciplinary, permanent staff uses our custom-tailored modeling tools for efficient CAMD-guided product and process development:

- quantitative structure-property relationships (QSPR)
- group contribution methods (GC)
- data mining methods
- molecular dynamics simulations (MD)
- monte carlo simulations (MC)
- quantum mechanical calculations
- computational fluid dynamics (CFD)

Our expertise comprises

- big data analysis
- design and optimization of new materials
- software development of simulation tools
- application of these tools to simulate polymers, biomolecules as well as molecular and ionic liquids
- professional knowledge transfer between university and industry

Properties that we can calculate include

density, molecule clustering, compressibility, excess volume, surface structure, self diffusion, viscosity, electrical/thermal conductivity, vapor pressure, lifetime of hydrogen bonds, octanol/water partition coefficient, heat of vaporization, heat capacity, solubility, surface tension

Fraunhofer Institute for Algorithms and Scientific Computing SCAI

Schloss Birlinghoven
53757 Sankt Augustin, Germany

Contact:
Dr. Jan Hamaekers
Head of Department
Phone +49 2241 14-2463
jan.hamaekers@scai.fraunhofer.de

Dr. Astrid Maaß
Phone +49 2241 14-2481
astrid.maass@scai.fraunhofer.de

www.scai.fraunhofer.de/vmd

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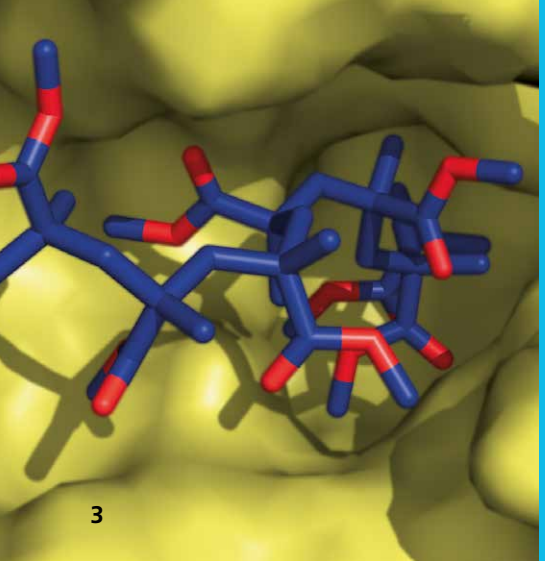
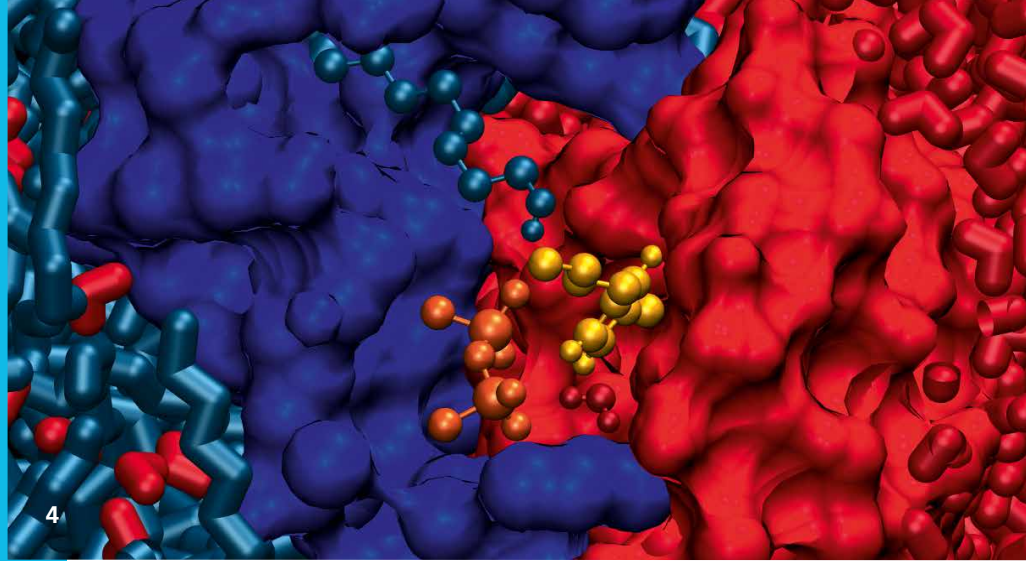
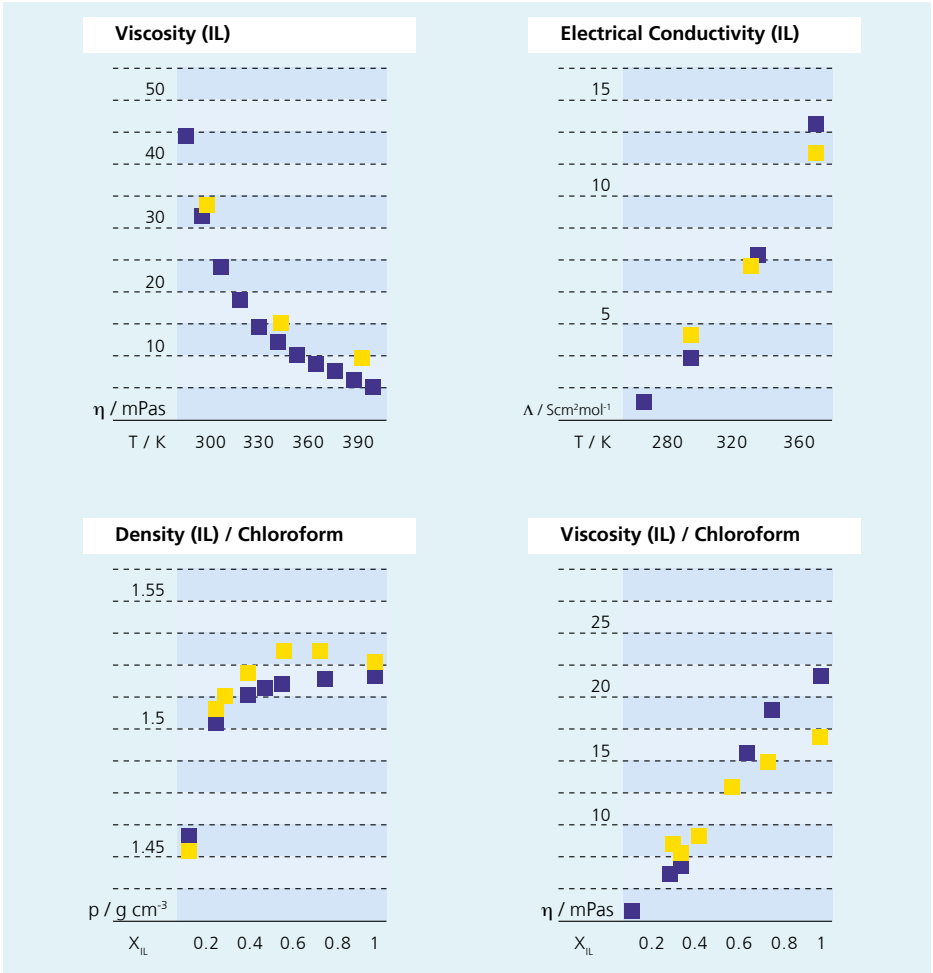




CAMD to develop ionic liquids (ILs)

Low-melting organic salts, commonly known as ionic liquids, have been of considerable interest to both scientific and industrial communities conducting their research in different fields of pure and applied chemistry since the beginning of the 1990s. Research focused on the discovery of new low-viscous ILs is crucial for the future development of ionic liquid science and technology. Searching for new ion structures can be performed by means of two methodologies. First, one can systematically (or by "hit-or-miss") check each possible cation-anion combination by direct experimental procedures, i.e. syntheses followed by measurements. Because of the huge number of ILs that one can imagine, such an approach is time consuming and thus expensive. The second method is based on CAMD. First of all, by using CAMD one can rapidly carry out comprehensive screenings of huge numbers of compounds without performing any experiments. Furthermore, the methodologies and models of CAMD can be built up on the basis of different ideas and mathematical tools. They can be derived either from theoretical ideas having physical foundations (e.g., molecular-based, thermodynamic), simple empirical correlations between viscosity and other thermophysical properties, generalized correlations, quantitative structure-property relationships (QSPRs), molecular simulations (MD, QMMD), or group contribution (GC) methods. The models can adopt simple linear or more complex nonlinear relationships between inputs (chemical information) and outputs (properties) as well as sophisticated machine-learning algorithms such as artificial neural networks (ANNs). In particular, QSPR correlations are developed on the basis of molecular descriptors obtained directly from chemical structure or input data that are experimental in nature. In turn, GC models use schemes to decompose the cation and anion moieties into arbitrarily defined functional groups. The set of structures used in the model development usually covers a certain fraction of the domain and is used to fit some parameters/constants that can eventually be adopted to predict the properties of other compounds.



3 *A PMMA atomistic model to investigate structure-property relationships.*

4 *Ionic liquid ion pair at the interface between water and octanol. Simulation of the octanol/water partition coefficient.*