Amsterdam Modeling Suite

Making Computational Chemistry Work for You

SCM
Software for Chemistry & Materials

The Amsterdam Modeling Suite

Powerful Computational Chemistry

Materials
Organic Electronics
Spectroscopy
Catalysis
Batteries
Polymers
Inorganic Chemistry
Heavy Elements
Oil & Gas
Nanoscience
Life Sciences
Bonding Analysis

Cutting-edge software

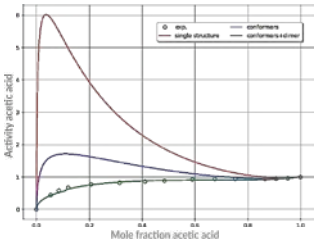
The Amsterdam Modeling Suite (AMS) is state-of-the-art computational chemistry & materials modeling software. Our developers focus on support and usability.

Proven since the early days of computational chemistry, AMS has grown into a versatile chemistry & materials modeling suite covering atomistic, kinetics, and fluid thermodynamics simulations.

Functionality

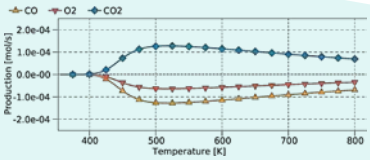
Selected compute engines

Continuum



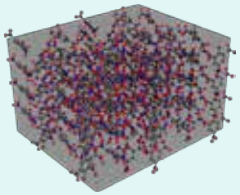
Fluid Thermodynamics
COSMO-RS
COSMO-SAC
UNIFAC

Mesoscale



Kinetics
Kinetic Monte Carlo
Microkinetics

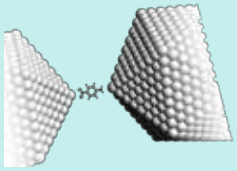
Materials



Force Fields
ReaxFF, GFN-FF
Machine Learning Potentials
Apple & P

QM/MM
FDE, Hybrid Engine

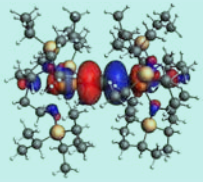
Nano



Tight binding
GFN-xTB, DFTB

Periodic DFT
BAND, Quantum Espresso

Atomistic



Molecular DFT
ADF

Materials

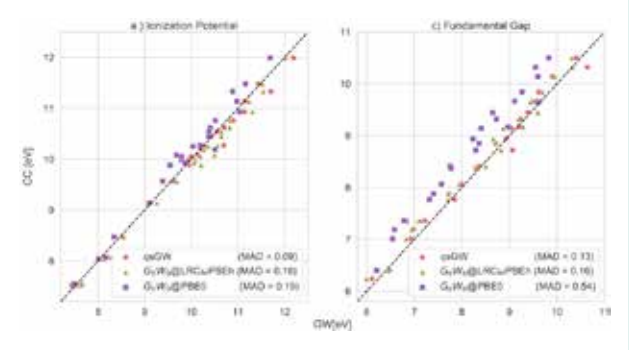
www.scm.com/applications/materials-science

Predict and understand materials properties from atomistic simulations with AMS: From molecular and periodic DFT to reactive molecular dynamics and fluid thermodynamics.

Your benefits

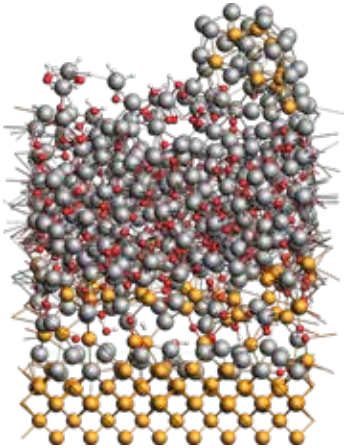
- Easily build clusters, nanotubes, crystals
- Workfunctions, electric fields, polarization, deposition processes treated naturally with real 2D surfaces
- ReaxFF: Many properties, acceleration techniques, and parametrization tools

Excellent predictions for ionization potential and fundamental gap with qsGW



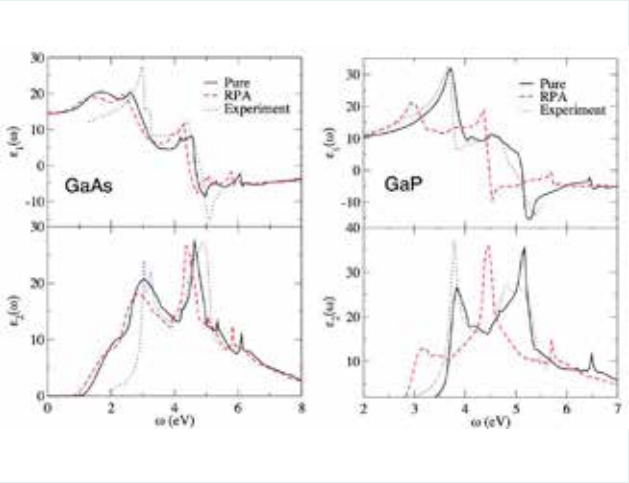
www.scm.com/qs-gw

Chemical Vapor Deposition of AlH3 on Ge(100) simulated with ReaxFF



www.scm.com/product/reaxff

Accurate optical spectra of semi-conductors and insulators with BAND



www.scm.com/semiconductor-spectra

Batteries & Photovoltaics

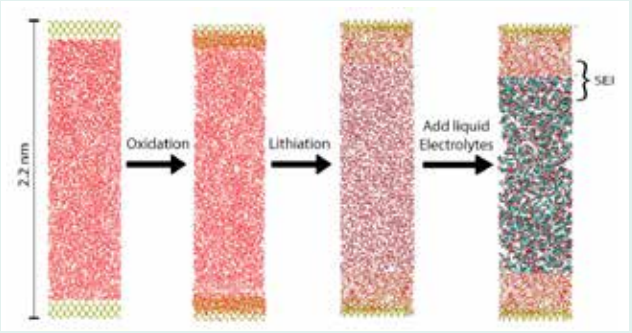
www.scm.com/applications/batteries

Simulate battery discharge processes with ReaxFF to understand and optimize charge mobility and reduce electrolyte decomposition. Screen electrode materials for desired band structures and accurately model surface-electrolyte interactions for detailed atomistic insight in electrochemical processes.

What can you model with AMS?

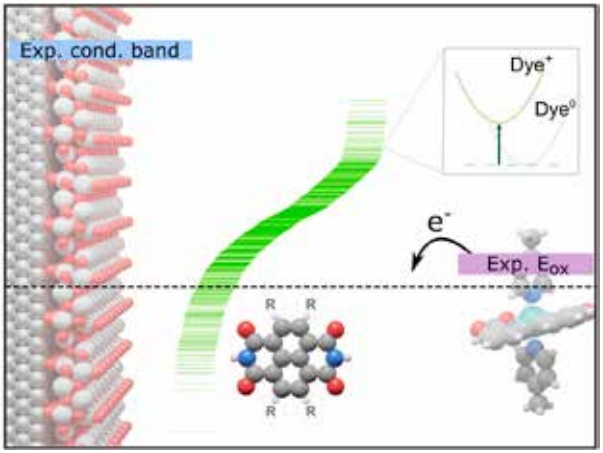
- Reactions, diffusion and charge transport
- Partial, local, full densities of states (DOS)
- Accurate relativistic treatments
- Advanced excited state properties (e.g. exciton coupling) for photovoltaics
- Improved band gaps with model potentials
- Easy orbital and density analysis
- Accurate mobilities for electrolytes with Apple&P polarizable force field
- Spectroscopic properties from NMR to XANES

SEI formation in Li-ion batteries with ReaxFF



www.scm.com/reaxff-sei

Screening redox potentials of dyes for photelectrochemical cells



www.scm.com/redox-screening

Organic Electronics

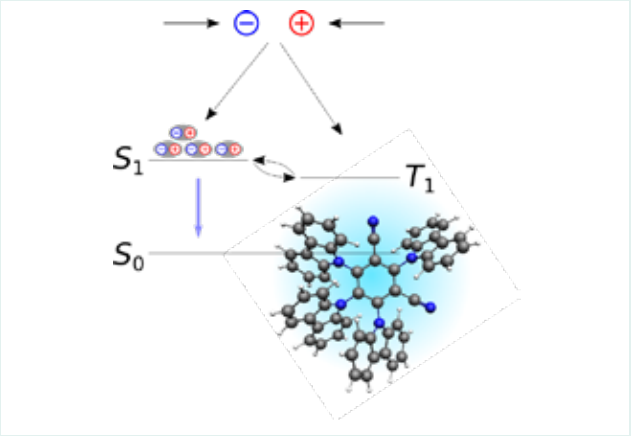
www.scm.com/organic-electronics

Optimize materials for organic electronic devices through atomistic modeling of materials. Improve emission, charge generation, charge transport and other properties in OLEDs, OFETs, and OPVs.

Selected Applications

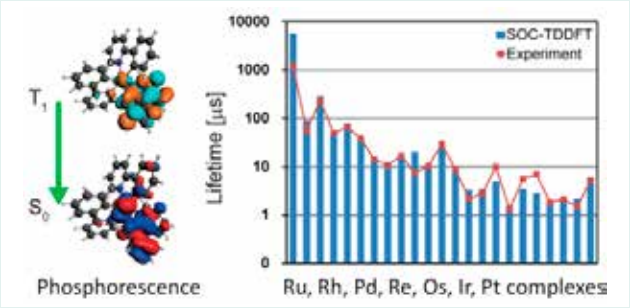
- Phosphorescence
- Charge transport
- Exciton coupling
- Charge transfer states with (tuned) range separated hybrids
- Accurate ionization potentials and electron affinities with qsGW
- Multiscale OLED workflows - from ab-initio atomistic to device level kinetic Monte Carlo

Tutorial: Thermally delayed fluorescence



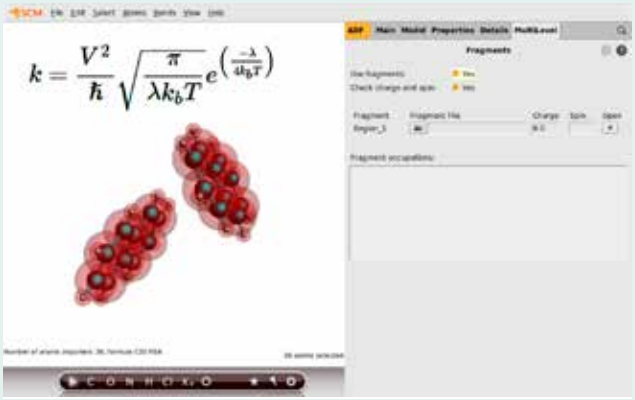
www.scm.com/tadf-tutorial

OLED phosphorescence with relativistic TDDFT



www.scm.com/oled_phosphorescence

Tutorial: Charge transfer integrals



www.scm.com/charge-transfer-integrals

Oil & Gas

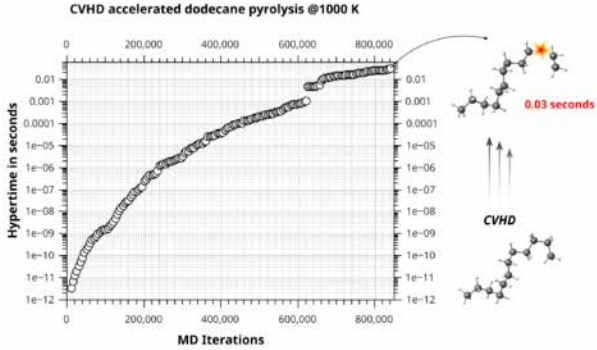
www.scm.com/applications/oil-and-gas

Study catalytic activation with DFT, combustion reactions with ReaxFF, or predict vapor-liquid equilibria with COSMO-RS.

How will AMS modeling help you?

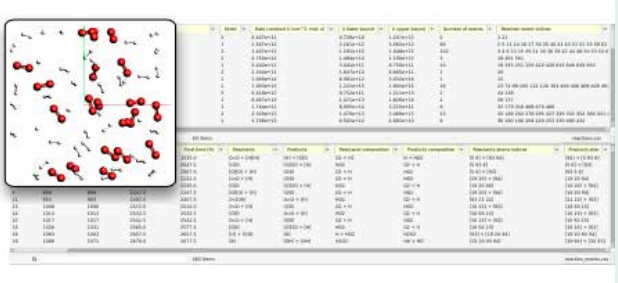
- Analyze combustion reaction networks / kinetics
- Accelerate reaction dynamics
- Bonding Analysis: Activation strain model for rational catalyst design
- Optimize solvents for extraction and other chemical processes

Tutorial: Collective-variable driven hyperdynamics



www.scm.com/cvhd

ChemTraYzer 2: Unique reactions and rate constants from MD trajectories



www.scm.com/ct2

Polymers

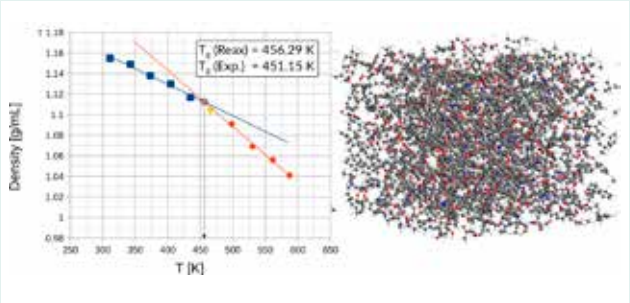
www.scm.com/applications/polymers

The Amsterdam Modeling Suite offers powerful computational chemistry tools to advance your polymer research projects.

How will AMS modeling help you?

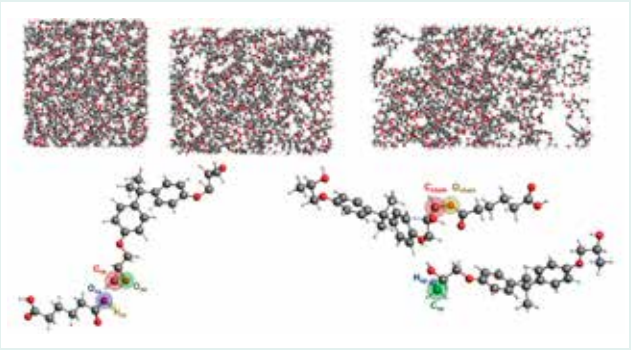
- Predict polymer cross-linking and degradation mechanisms
- Stress/strain and failure mechanisms of polymers and composites
- Predict glass transition temperatures, thermal expansion coefficients
- Design optimal solvent mixtures to dissolve your polymers
- Study catalytic polymerization
- Predict important thermodynamic properties for polymer/solvent and polymer/polymer systems

Tutorial: Glass transition temperature of a thermoset polymer



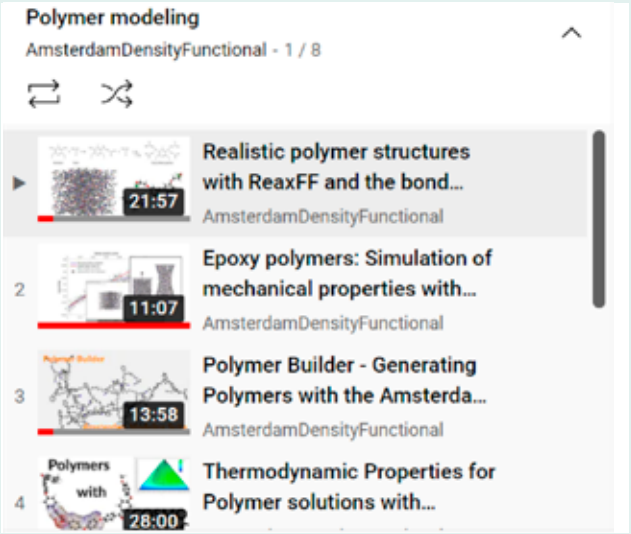
www.scm.com/glass-trans-temp

Reversing fatigue in carbon-fiber reinforced vitrimer composites



www.scm.com/self-healing-polymers

AMS polymer modeling playlist



www.scm.com/polymer-playlist

Life Sciences

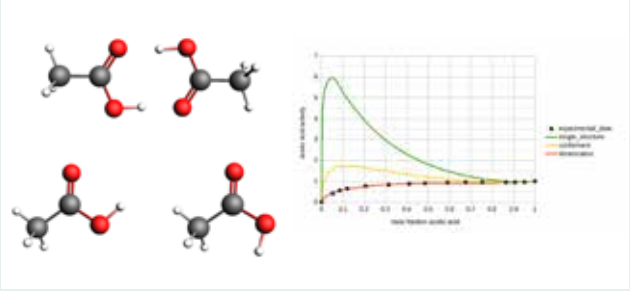
www.scm.com/applications/pharma

Study ligand binding, conformations, and absolute configuration with ADF. Use COSMO-RS to quickly reduce the solvent mixture search space for recrystallization, improving solubility with excipients or purifying active pharmaceutical ingredients.

Boost your research

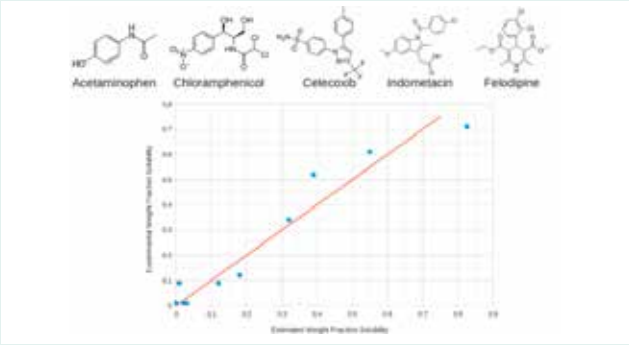
- Solubilities, logP, pKa, VLE, etc. based on DFT + thermodynamics
- Solvent optimization, e.g. for liquid-liquid extraction or recrystallization
- Accurate NMR predictions and analysis
- VCD analysis tools
- Accurate energies of organic crystals with DFTB+D

COSMO-RS with multi-species components



www.scm.com/multispecies-cosmo-rs

Instantaneous prediction of solubilities



www.scm.com/cosmo-rs-solubilities

Solvent optimization for solubility and liquid-liquid extraction

www.scm.com/solvent-optimization

Nanotechnology

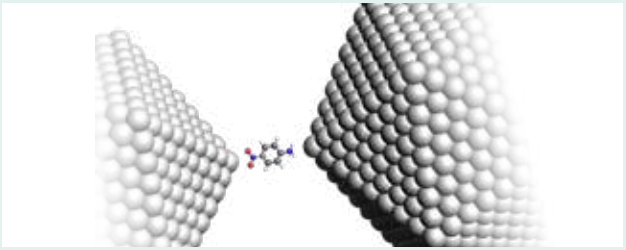
www.scm.com/applications/nanotechnology

Predict optical properties of quantum dots and other nanoparticles with the fast & accurate methods in ADF. Prescreen even more quickly with DFTB. Understand nanoparticle formation and other reactive processes at the nanoscale with ReaxFF.

Selected Features

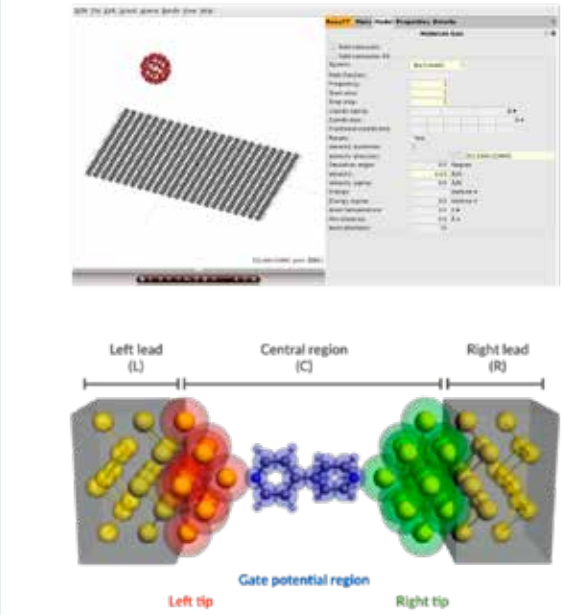
- Accurate relativistic effects with ZORA
- Frozen density embedding for environment effects and large systems
- Efficient and flexible embedding scheme (QM/QM',QM/MM,MM/MM) via hybrid engine.
- Fast TD-DFT with Model Potentials (SAOP, LB) and many spectroscopic properties
- 1000s of atoms with (TD)DFTB and Millions of atoms with ReaxFF

Tutorial: Plasmon-enhanced non-linear optical properties



www.scm.com/dim-qm-non-linear

ADF Powerful GUI to run and analyze calculations



www.scm.com/gui

Inorganic Chemistry

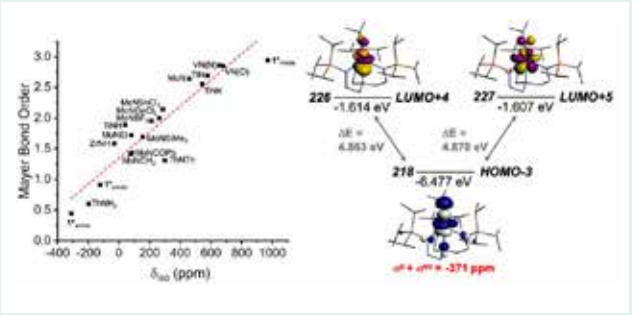
www.scm.com/applications/inorganic-chemistry

ADF and BAND are well suited for studying inorganic compounds: transition metal and organo-metallic complexes or systems with heavy elements. Fast, robust and accurate tight-binding method, GFN1-xTB, for structures and vibrational frequencies for all elements (Z=1-86).

Selected Features

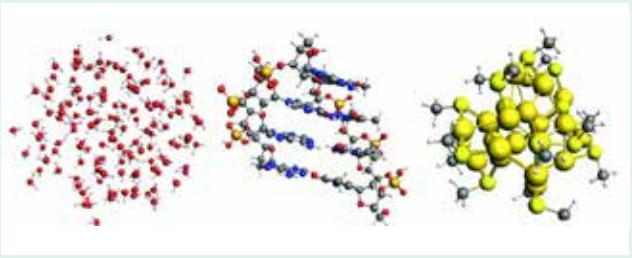
- From NMR to X-ray: Many spectroscopic properties
- Unique chemical bonding analysis
- Scalar-relativistic and spin-orbit coupling
- Slater-type all-electron, basis sets for all elements
- Robust SCF convergence methods

Exceptional Uranium-Nitride Triple Bond Covalency



www.scm.com/uranium-nitride-triple-bond

Double hybrid calculations for very large systems



www.scm.com/double-hybrids

ParAMS: Powerful parametrization toolkit

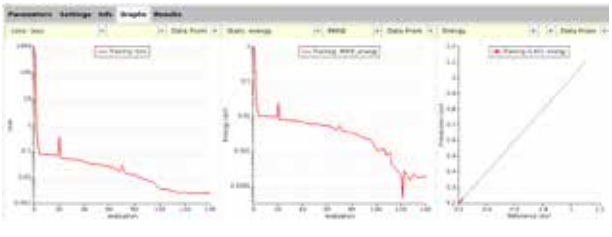
www.scm.com/params

Our powerful parametrization toolkit ParAMS enables you to parametrize ReaxFF and DFTB with full GUI support and an extensive Python library for customization.

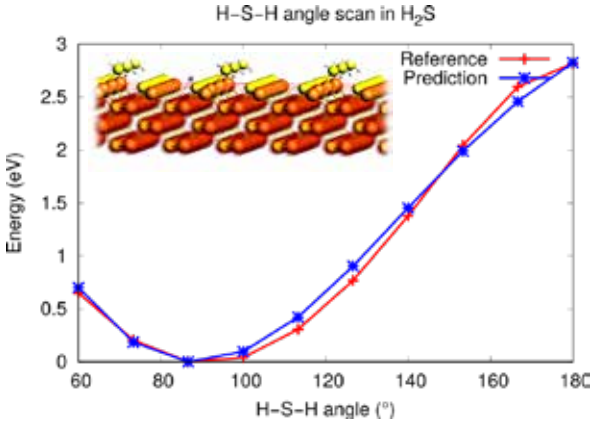
Highlights

- Easily import, build, and visualize training data sets
- Use data from AMS, VASP, Quantum ESPRESSO, and experiments
- Properties: energies, forces, geometries, stress tensors, charges, and many more...
- Use of validation sets to prevent overfitting
- Walk-through tutorials for real-life ReaxFF and DFTB use cases

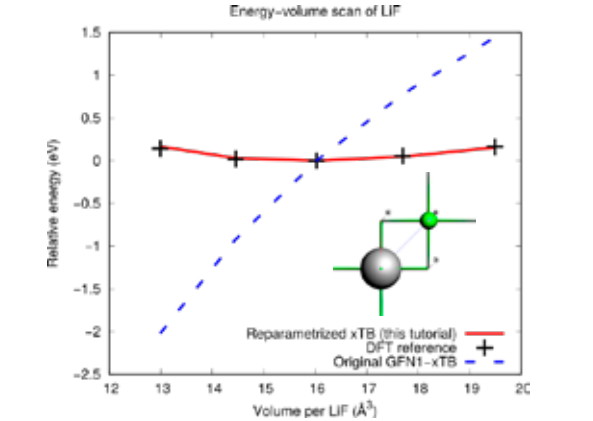
Full GUI support at every stage of the fitting workflows



ReaxFF Tutorial: Parametrization of ZnS and H_2S on ZnS(110)



GFN1-xTB Tutorial: Refitting of repulsive terms with ParAMS corrects Li-F interactions

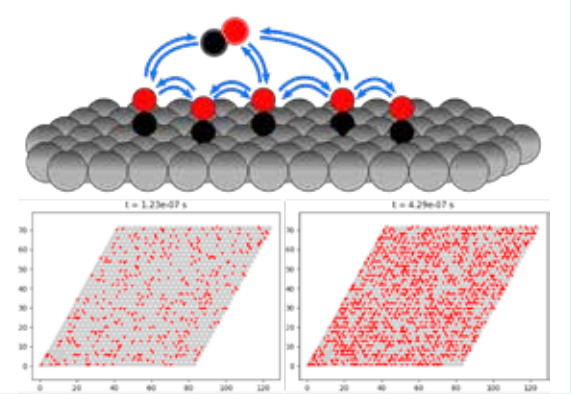


Reaction discovery and kinetics

From atomistic to mesoscopic modeling

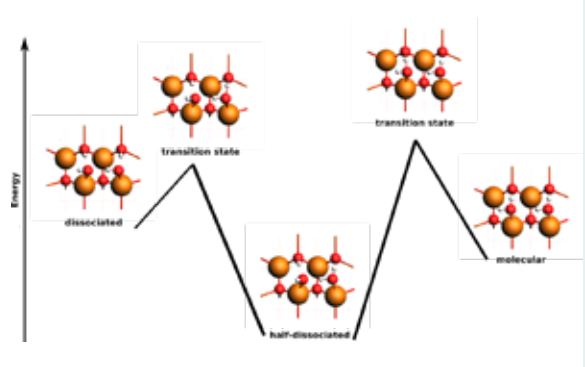
pyZacros/Zacros

Reactions on catalytic surfaces with kinetic Monte Carlo



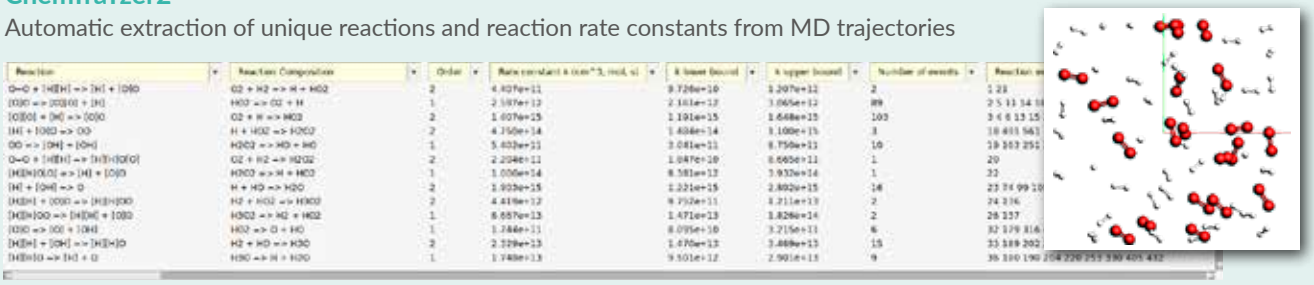
Automated PES Exploration

Automatic search for saddle points and local minima on any Potential Energy Surface



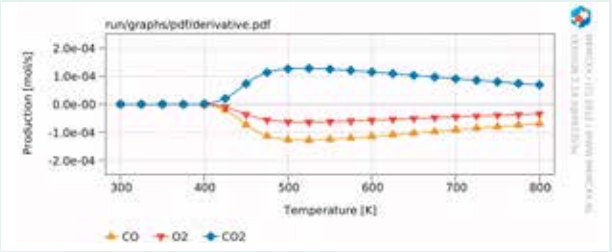
ChemTraYzer2

Automatic extraction of unique reactions and reaction rate constants from MD trajectories



MKMCXX Microkinetics

Reaction rates and rate limiting factors from elmentary reactions



Getting started

www.scm.com/support

Get started right away with our easy to follow step-by-step tutorials. From drawing and optimizing an ethanol molecule to fitting a ReaxFF force field or running an OLED workflow, there's a tutorial waiting.

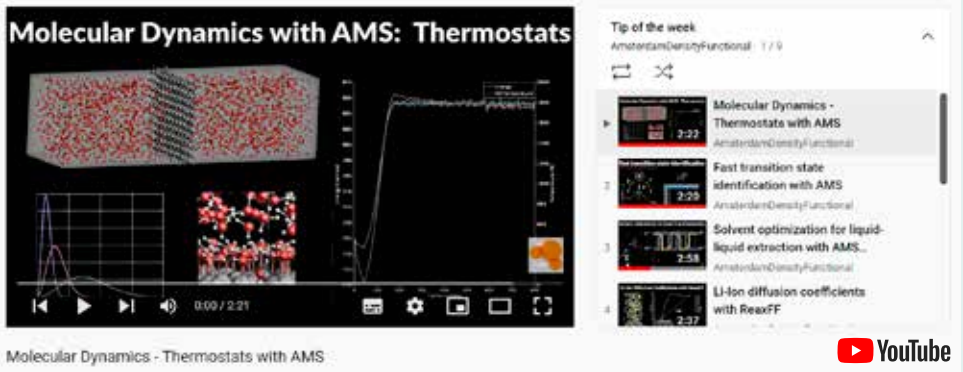
Easy start

- Online tutorials
- Videos
- Webinars
- Mailing list
- Expert technical support
- Custom tutoring, Consulting, Contract research

Tutorials

www.scm.com/tutorials

Videos



www.scm.com/video-tip-of-the-week

Contact us

www.scm.com

About us

Scientists at SCM are passionate about making computational chemistry work for you. Our mission is to develop powerful, easy-to-use software for your research and development needs.

We always value feedback on how to further improve our software in terms of capabilities, speed and usability! Not sure if a certain property can be modeled? Contact us and find out!

info@scm.com

Pricing

www.scm.com/price-quote/

Resellers

Our regional resellers offer first-line support for the Amsterdam Modeling Suite in the local language.

CHINA: 费米科技（北京）有限公司 www.fermitech.com.cn/ams/
技术支持 : support@fermitech.com.cn

JAPAN: www.molsis.co.jp/ams/
Dr. Kouji Chiba – sales@molsis.co.jp

KOREA: www.tnjtech.co.kr/v4/
Dr. Youngdae Joo – comj@tnjtech.co.kr

OTHER: www.scm.com/ams-resellers