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

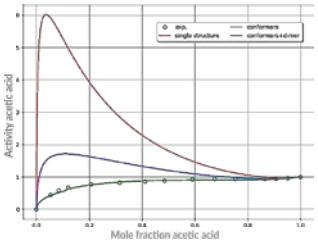
The Amsterdam Modeling Suite (AMS) is state-of-the-art computational chemistry & materials modeling software. Our developers focus on support and usability.

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.

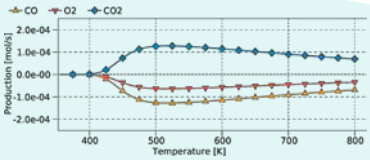
Functionality

Selected compute engines

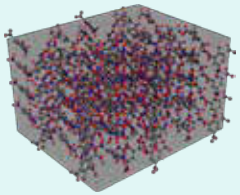
Continuum



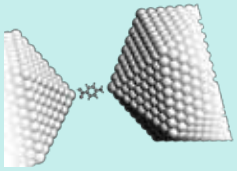
Mesoscale



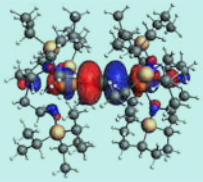
Materials



Nano



Atomistic



Fluid Thermodynamics
COSMO-RS
COSMO-SAC
UNIFAC

Kinetics
Kinetic Monte Carlo
Microkinetics

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

QM/MM
FDE, Hybrid Engine

Tight binding
GFN-xTB, DFTB

Periodic DFT
BAND, Quantum Espresso

Molecular DFT
ADF

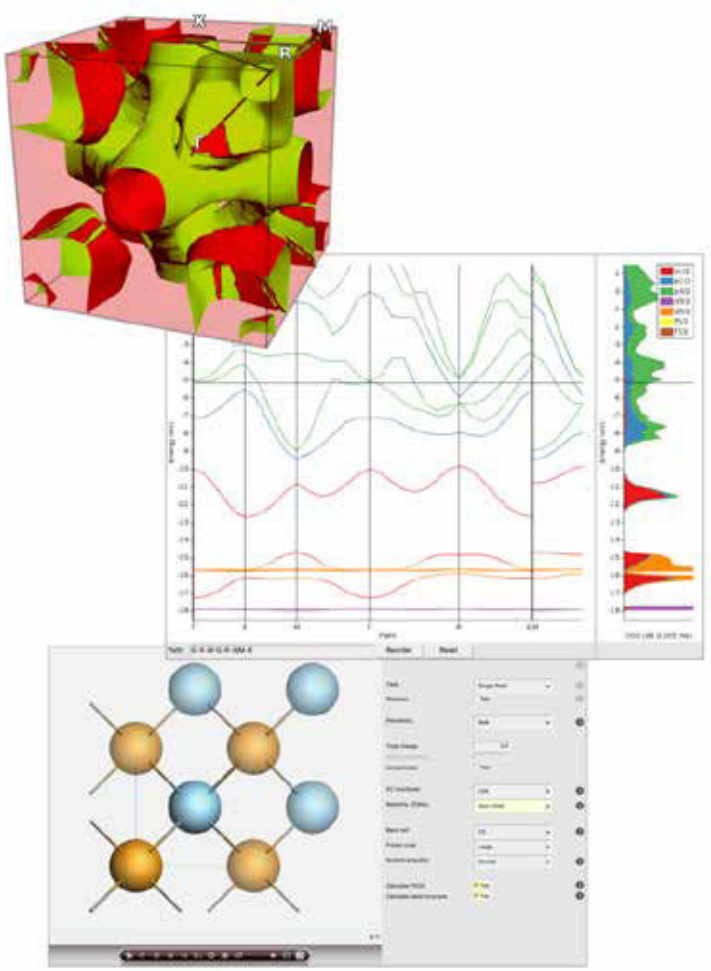
Materials Science

www.scm.com/applications/materials-science

Predict and understand materials properties from atomistic simulations with **AMS**. From periodic DFT for nanotubes, surfaces and bulk (**BAND, Quantum Espresso, ASE engines**) to reactive molecular dynamics simulations with **ReaxFF** and **Machine Learning** potentials.

What can you do with AMS?

- Extract accurate materials properties including work functions, optical spectra, ionization potentials, bandgaps, etc.
- Model physical processes based on large scale atomistic simulations of sputtering, etching, and chemical vapor deposition
- Study the mechanical properties of materials with automatic **workflows** for Young's modulus, yield point, Poisson's ratio, and tribology calculations
- Discover new materials with **M3GNET**, the new universal machine learning potential
- Create novel **ReaxFF** or **DFTB** parameter sets that suits your needs with **ParAMS**



Band structure & DOS of TlBi with BAND

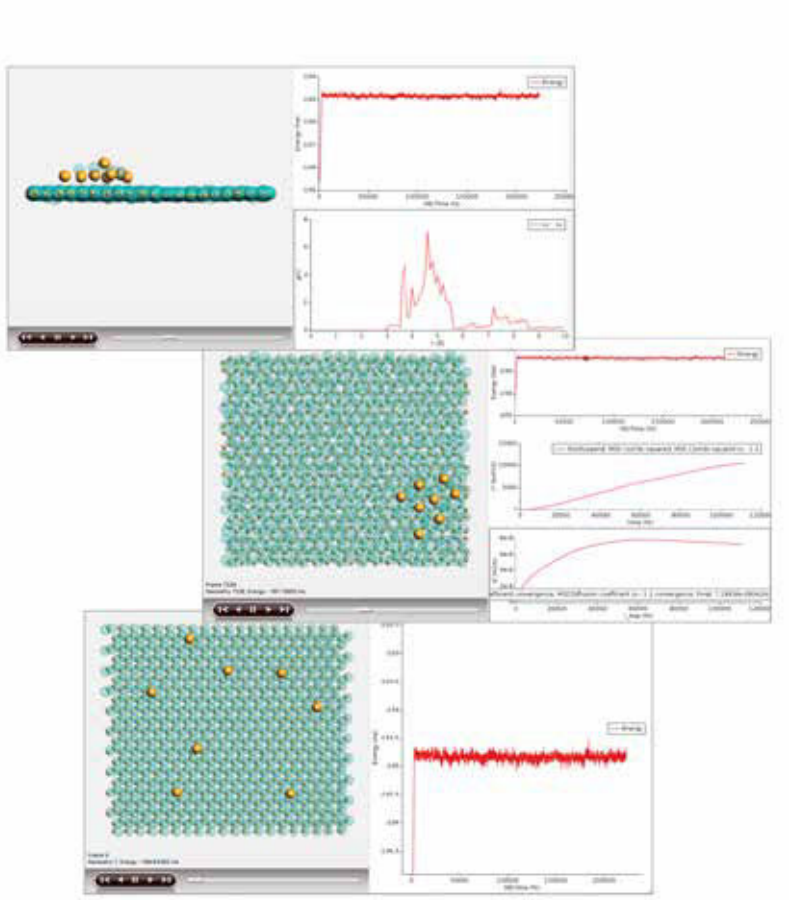
Batteries & Photovoltaics

www.scm.com/applications/batteries

Accelerate R&D, reduce cost, environmental impact and safety of batteries and photovoltaics. From fundamental molecular properties to large scale reactive simulations of interfaces with explicit electrons.

What can you do with AMS?

- Model reactions, diffusion, nucleation (Li-plating, SEI) and charge transport with **ReaxFF** and **eReaxFF** (explicit electrons)
- Screen materials to target properties (bandgaps, redox potentials)
- Optimize electrolyte properties (mobility, viscosity, conductivity, solubility) with polarizable force field (**Apple&P**) and continuum models (**COSMO-RS**)
- Predict spectroscopic properties with advanced solvation/environments (NMR, EPR, UV, XAS)



Li plating on graphene with eReaxFF

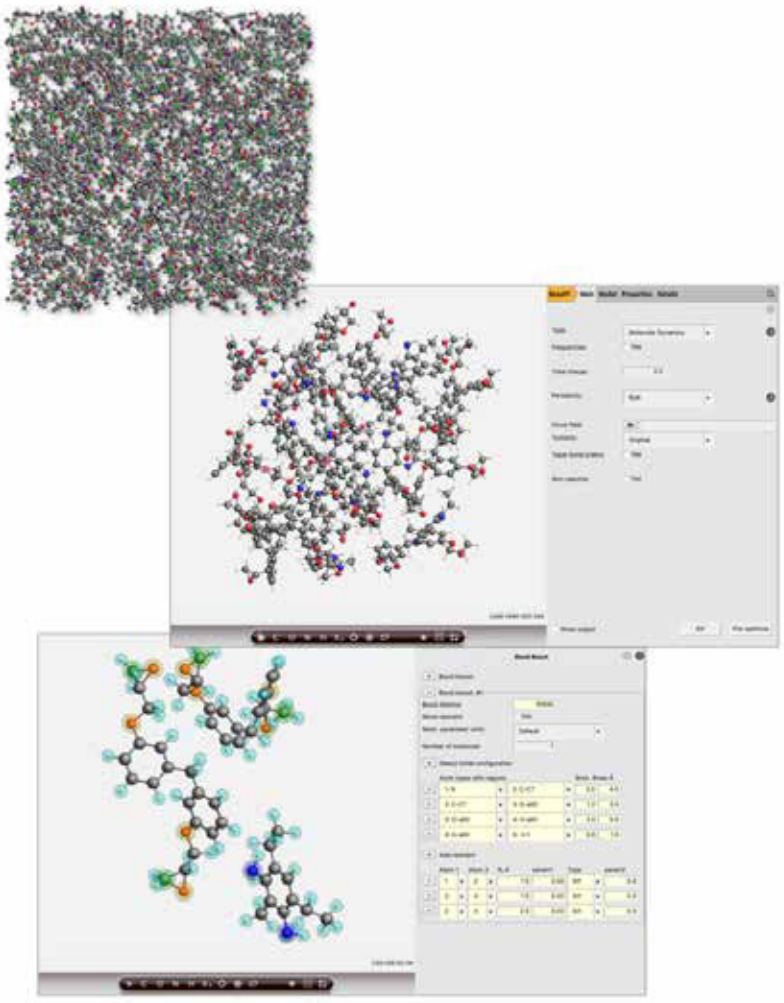
Polymers

www.scm.com/applications/polymers

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

What can you do with AMS?

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



Modeling cross-linked polymer with ReaxFF & Bond boost

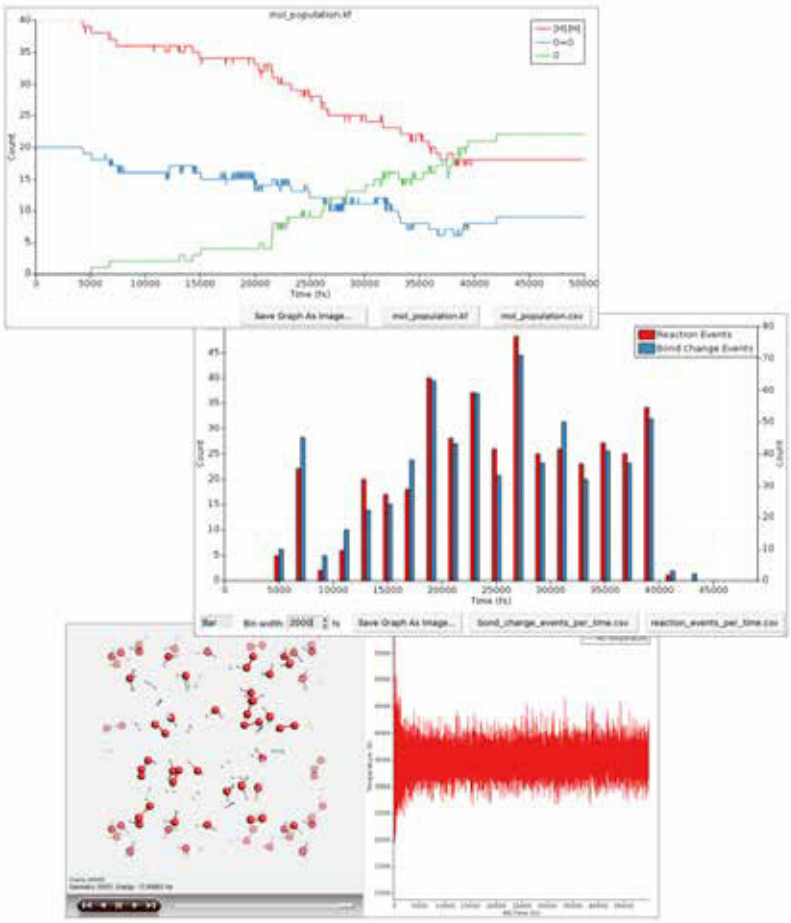
Oil & Gas

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

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

What can you do with AMS?

- Analyze combustion reaction networks and kinetics (**ChemTraYzer 2**)
- Accelerate reaction dynamics into millisecond timescale (hyperdynamics) and automate potential energy surface exploration
- Analyze bonding with activation strain model for rational catalyst design
- Optimize solvents for extraction and other chemical processes
- Screen catalysts for activity with **kinetic Monte Carlo (pyZacros/Zacros)**
- Study complex combustion reactions



Combustion reaction with ReaxFF analyzed with ChemTraYzer 2

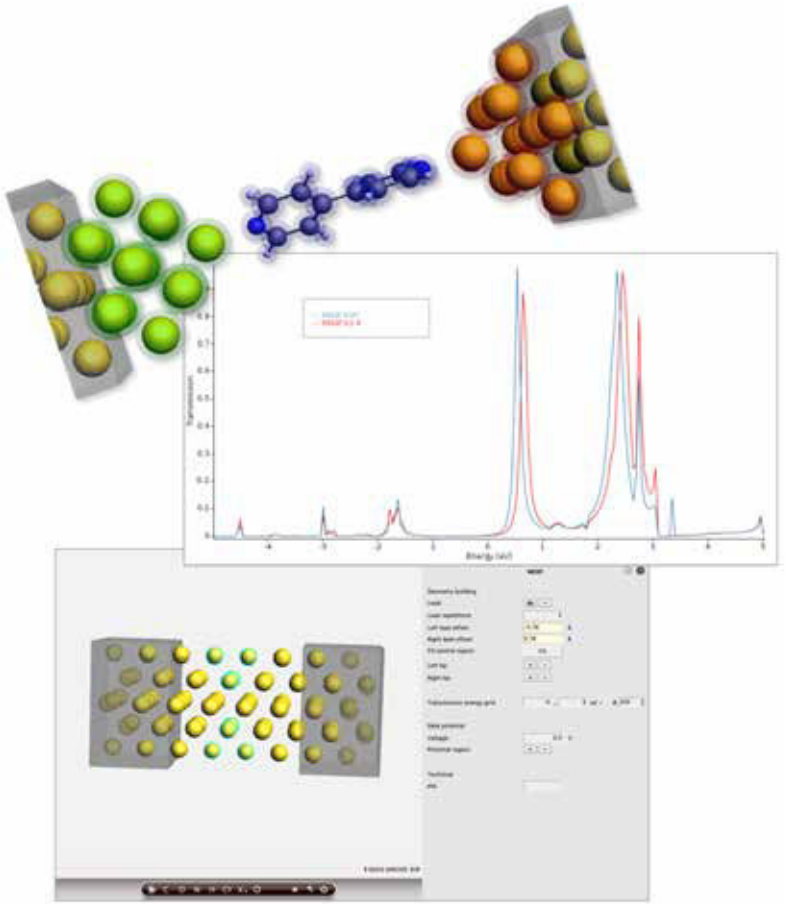
Nanotechnology

www.scm.com/applications/nanotechnology

With our molecular and periodic DFT codes (**ADF** and **BAND**), study nanoparticles and molecular junctions with accurate treatment of relativity (**ZORA**), fast **TDDFT** methods, and specialized exchange-correlation potentials. Advanced methods are available for environments and multilevel calculations.

What can you do with AMS?

- Predict optical properties of quantum dots and other nanoparticles with **ADF**
- Simulate electronic transport with non-equilibrium Green's function (**NEGF**)
- Compute spectroscopic properties with **TDDFT**
- Model realistic nano-objects with our efficient and flexible embedding scheme via **hybrid engine** (QM/QM', QM/MM, etc.)
- Understand nanoparticle formation and reactive processes with **ReaxFF**



Plasmon enhanced two photon absorption with ADF & NEGF

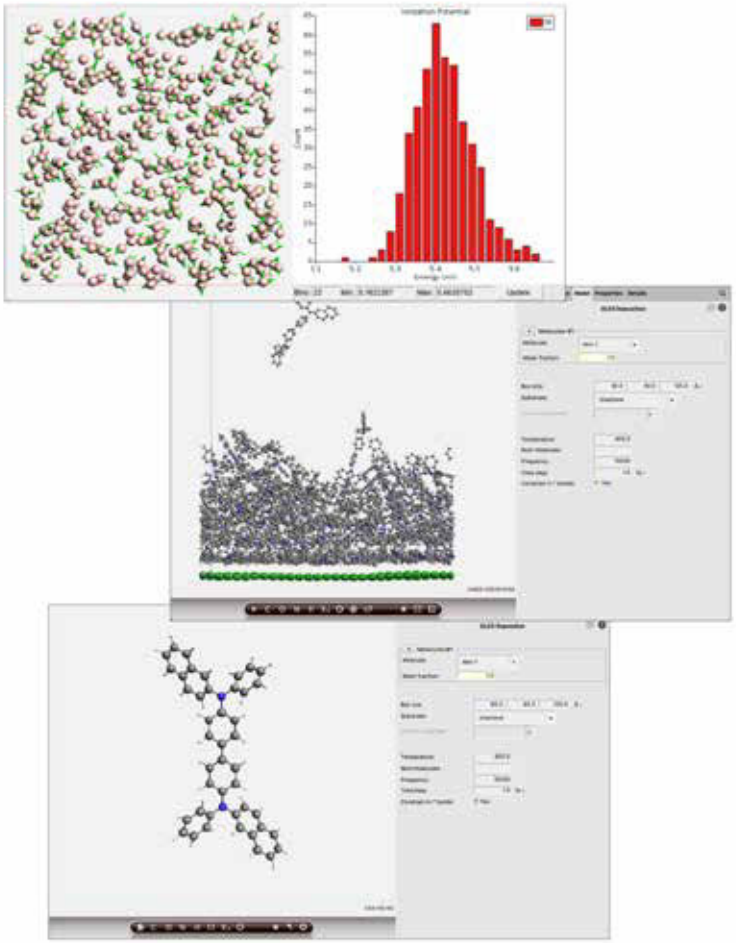
Organic Electronics

www.scm.com/organic-electronics

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

What can you do with AMS?

- Optimize OLED emission lifetimes and colors with spinorbit **TDDFT**
- Accelerate materials discovery with high-throughput prediction of OLED properties based on molecular structure
- Predict charge mobility, charge transport, exciton coupling, ionization potentials, electron affinities, etc.
- Perform multiscale workflows from ab initio atomistic to **kinetic Monte Carlo**
- Model large scale deposition (sputtering, etching) with **DFTB, ReaxFF** and **Machine Learning** potentials



Multiscale modeling of OLED with AMS workflow

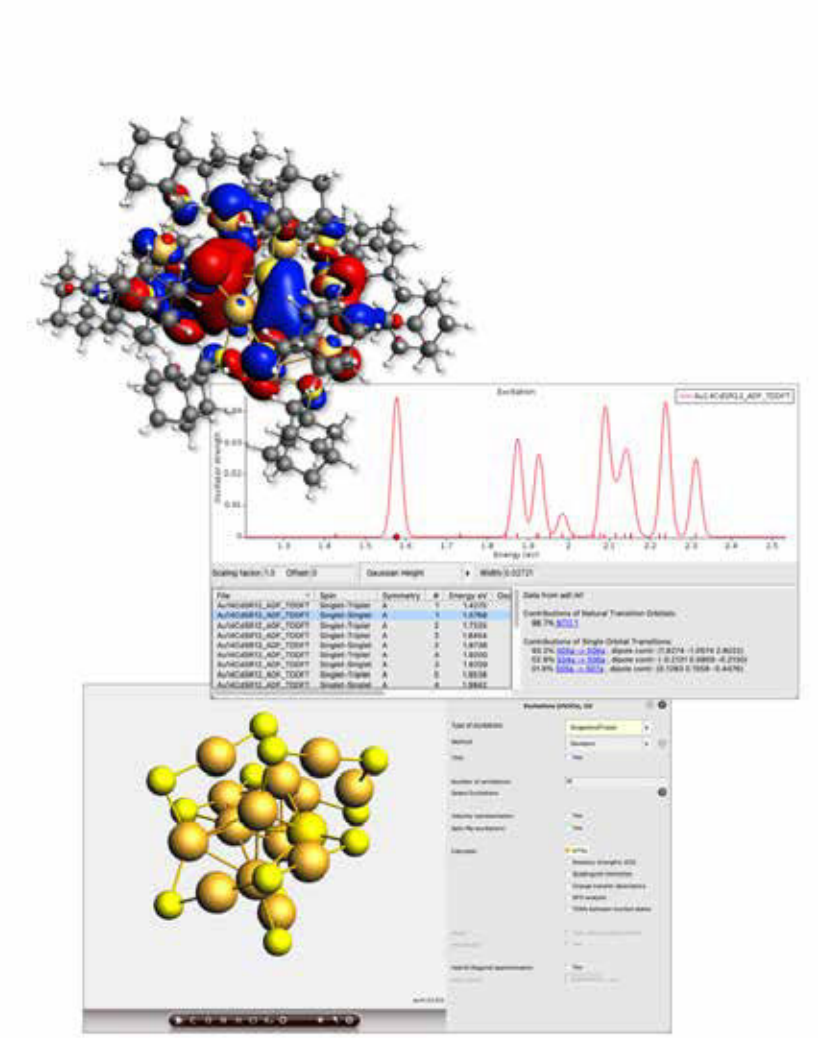
Inorganic Chemistry

www.scm.com/applications/inorganic-chemistry

ADF is a powerful density functional theory code for studying inorganic compounds, such as transition metal and organometallic complexes. Relativistic effects are accurately and efficiently treated with the **ZORA** Hamiltonian for heavy elements.

What can you do with AMS?

- Compute accurate (GW, spin orbit) spectroscopic properties from NMR chemical shifts to X-Ray spectra
- Analyze chemical bonding with various orbital decomposition schemes (EDA, ETS, NOCV)
- Visualize energy level diagrams and orbitals
- Calculate excitation energies, oscillator strengths, polarizabilities, CVD spectra, magnetizabilities, band gaps etc., using TDDFT
- Study large organic complexes efficiently with fast and accurate approximations (PolTDDFT, TDDFT+TB)

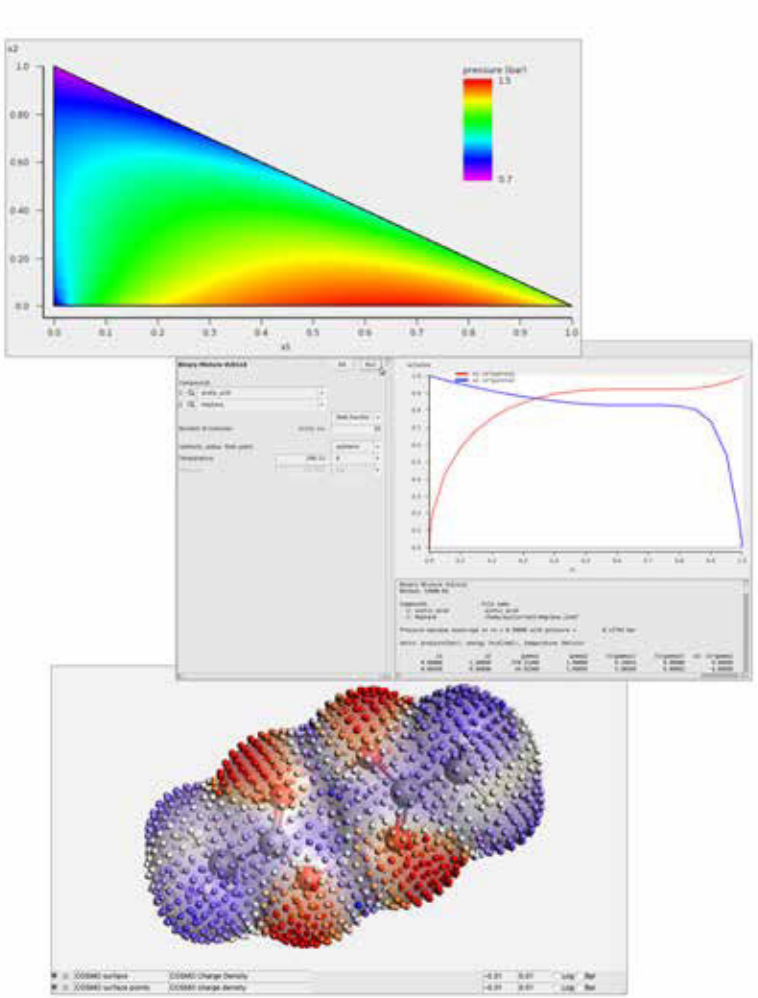


UV/Vis spectra of Au14CdSR12 with TDDFT

Life Sciences

www.scm.com/applications/pharma

Boost your pharma research with AMS' complete multi-scale tools. Study ligand bonding, conformations, and absolute configuration with DFT. Use **COSMO-RS** to quickly reduce the solvent mixture search space for recrystallization, improving solubility with excipients or purifying active pharmaceutical ingredients.



What can you do with AMS?

- Predict solubilities, logP, pKa, VLE, etc. based on DFT + thermodynamics (**COSMO-RS**)
- Optimize solvents, e.g. for liquid-liquid extraction or recrystallisation
- Analyze and predict NMR and VCD spectra with **ADF** and AMS spectra/VCD tools
- Extract accurate energies of organic crystals with **DFTB**
- Perform large scale simulations with reactive force fields and **Machine Learning** potentials for biochemistry
- Search for conformers and refinement with **RDKit** and **CREST**

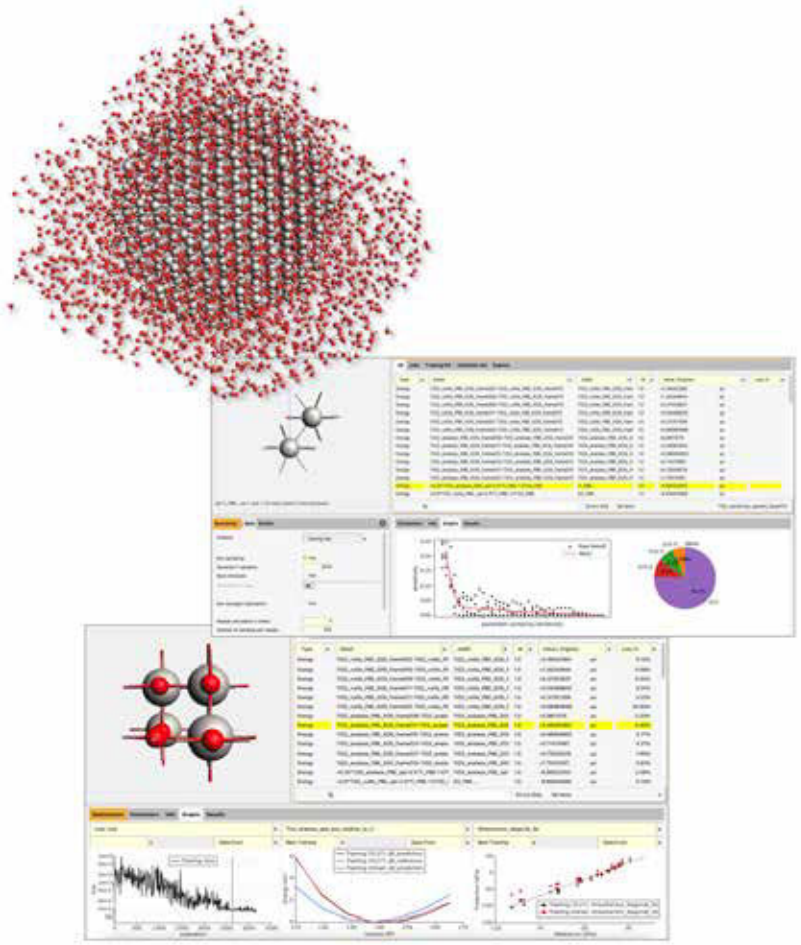
Parametrization toolkit

www.scm.com/applications/params

Create your own atomistic models to describe novel materials and molecules. With ParAMS you can easily develop ReaxFF and DFTB parameter sets with full support of the graphical user interface and Python library for advanced customization.

What can you do with ParAMS?

- Import, build and visualize training sets
- Use data from **AMS, VASP, Quantum Espresso**, and experiments
- Tune parameters to describe properties such as energies, forces, geometries, stress tensors, charges, bandgaps, band structure, etc.
- Use validation sets to prevent overfitting
- Submit multiple optimizations at the same time to explore parameters space
- Explore the sensitivity of the parameters to select the most meaningful subset to optimize



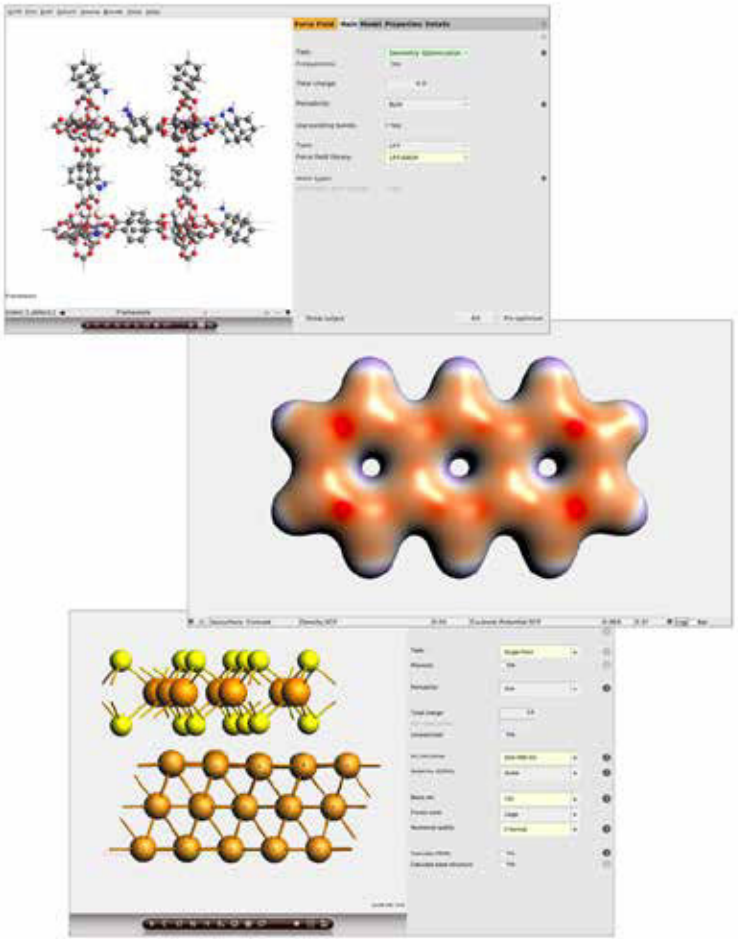
The graphical user interface

www.scm.com/applications/gui

With the graphical user interface you can access all engines in AMS and perform advanced simulations in a simple and intuitive approach. It will boost your productivity whether you are a beginner or a seasoned computational chemist. The GUI is cross platform (Linux, Windows and MacOS) and also provides interfaces to VASP and Quantum ESPRESSO.

What can you do with the GUI?

- Build molecules, periodic systems, polymers, and import structures from all major file formats
- Manage your jobs, locally or remotely to a cluster computer
- Analyze the results of your simulations (MSD, autocorrelation functions, histograms)
- Extract summaries of your calculations in structured data files (xlsx, csv)
- Visualize structures, transition states, orbitals, densities, DOS, band structures, spectra, energy landscapes, fitting results, etc.



Snapshots of the GUI for various applications

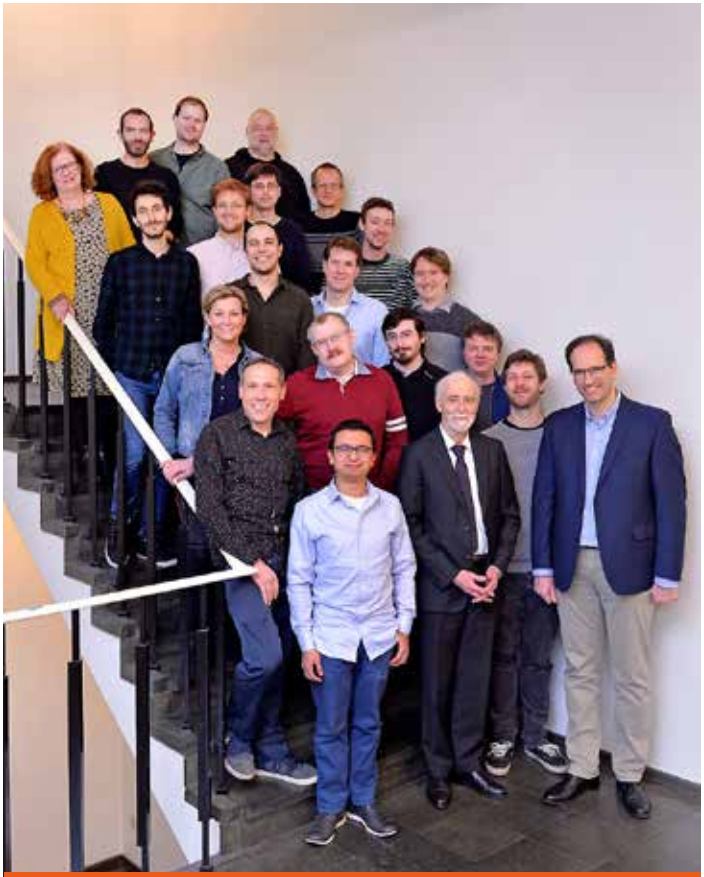
Getting started

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 a multi-scale OLED workflow, there is a tutorial waiting for you.

Easy start

- Extended documentation
- More than 100 tutorials, and tutorial series on industry relevant topics
- Videos and webinars
- Expert technical support
- Custom tutoring, consulting and contract research



The SCM team

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