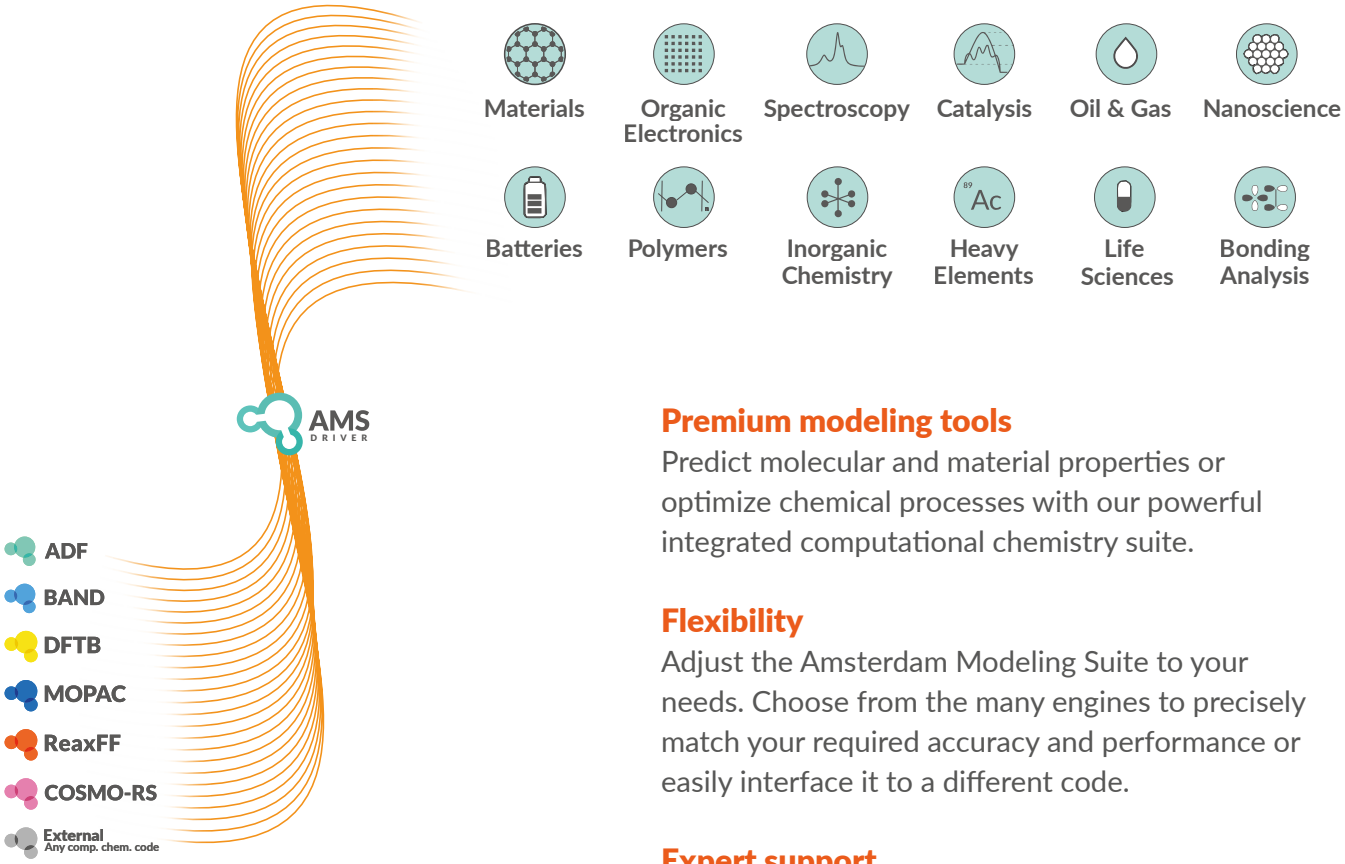
Amsterdam Modeling Suite

Making Computational Chemistry work for you

SCM
Software for Chemistry & Materials

The Amsterdam Modeling Suite

Powerful Computational Chemistry



Premium modeling tools

Predict molecular and material properties or optimize chemical processes with our powerful integrated computational chemistry suite.

Flexibility

Adjust the Amsterdam Modeling Suite to your needs. Choose from the many engines to precisely match your required accuracy and performance or easily interface it to a different code.

Expert support

Learn how to apply the latest computational materials workflows from our step-by-step online tutorials and receive expert technical support directly from the AMS developers.

The AMS concept

Key to flexibility

The AMS driver is a powerful tool to quickly set up advanced molecular dynamics and potential energy surface tasks with any atomistic code.

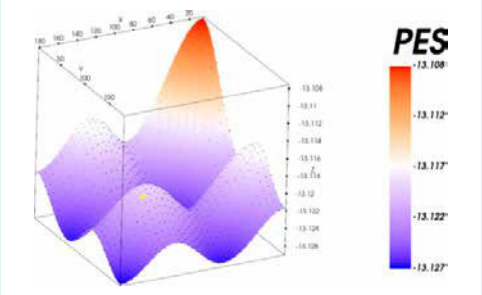
Quickly find minima or transition states and seamlessly switch to a more accurate method with the AMS driver.
Run advanced MD or MC simulations with any computational engine.
Calculate (selected) frequencies, phonons, and elastic tensors.

How will the AMS driver help you?

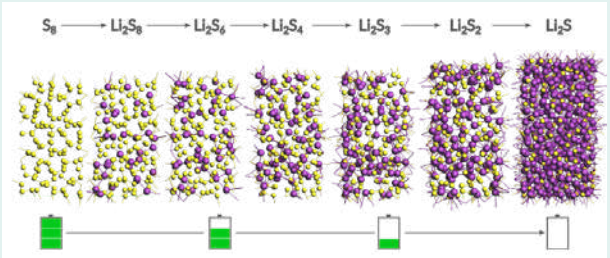
With any computational engine, easily do:

- Robust geometry optimization
- Advanced PES tasks
- Sophisticated MD ensembles
- Monte Carlo and molecule gun
- Many static & dynamic properties
- Script workflows with PLAMS

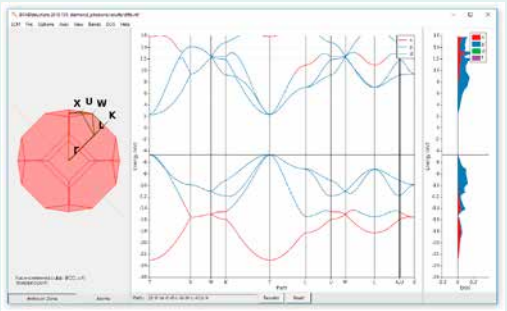
Advanced PES scans



Molecular dynamics ensembles, Monte Carlo, Acceleration Techniques



Frequencies, Phonons, Stress and Elastic Tensors,...



Materials

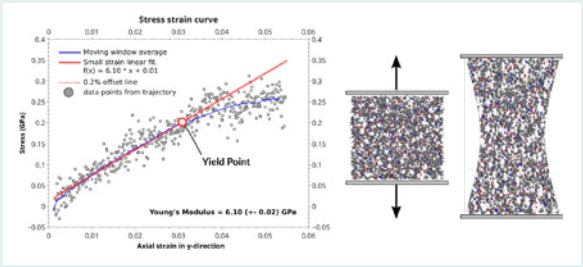
www.scm.com/applications/materials-science/

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

Your benefits

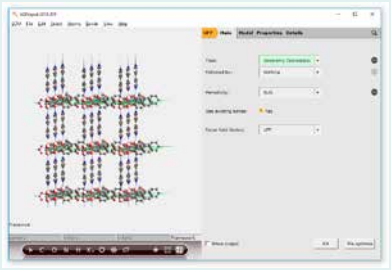
- Easily build clusters, nanotubes, crystals
- Molecular and periodic DFT
- Proper 2D representation for surfaces with BAND, MOPAC, and DFTB
- ReaxFF: Many properties, acceleration techniques, and parametrization tools

Mechanical Properties of Polymers



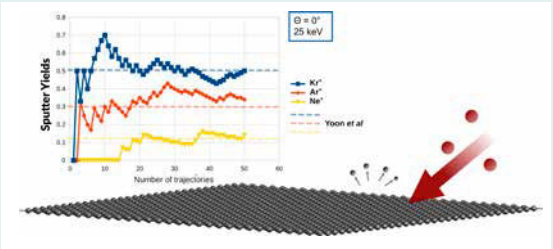
www.scm.com/epoxide-modeling

Framework Builder in the GUI



www.scm.com/mof-cof-builder

Molecule Deposition, ALD, CVD & Sputtering



www.scm.com/molecule-gun

Organic Electronics

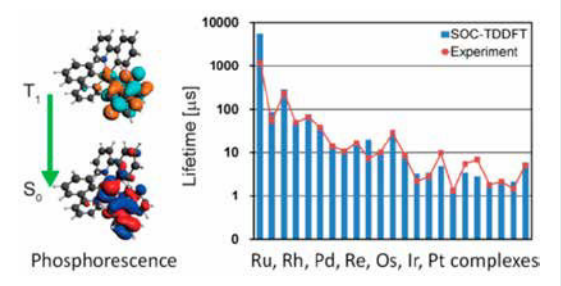
www.scm.com/organic-electronics/

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.

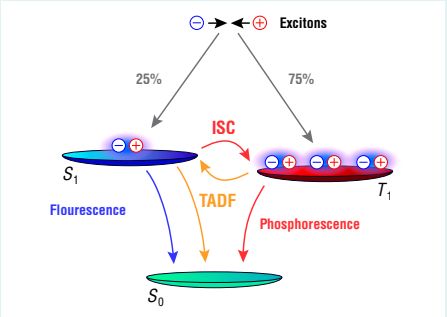
Selected Applications

- Phosphorescence
- Charge transport
- Exciton coupling
- Charge transfer states with (tuned) range separated hybrids

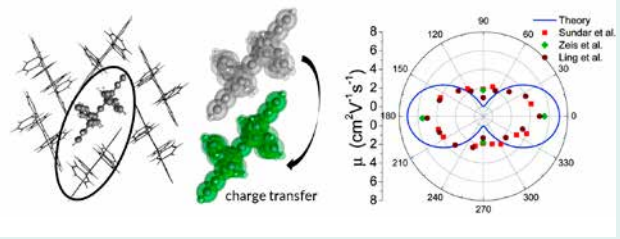
Phosphorescence Lifetimes of OLED emitters



Thermally Activated Delayed Fluorescence (TADF)



Hole/Electron mobility in OFETS



www.scm.com/organic-electronics/

Batteries & Photovoltaics

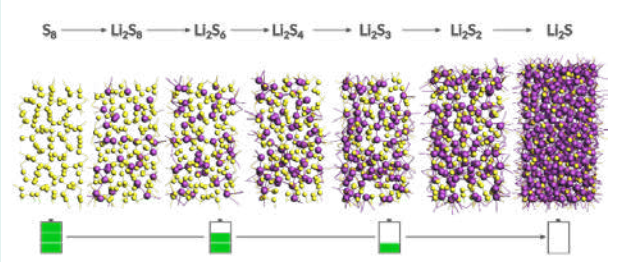
www.scm.com/applications/batteries/

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 electro-chemical processes.

What can you model with AMS?

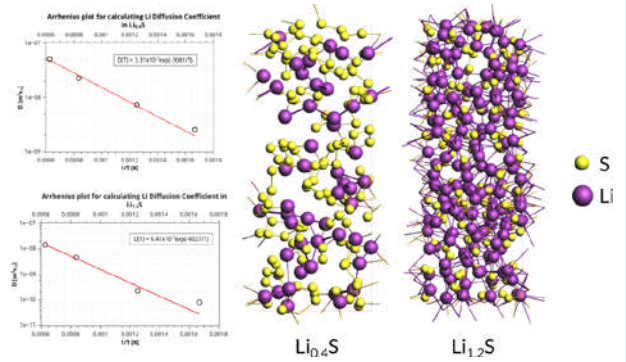
- Reactions, diffusion and charge transport
- Partial, local, full densities of states (DOS)
- Accurate relativistic treatments
- Advanced excited state properties (e.g. exciton coupling) for photovoltaics
- Improved band gaps with model potentials
- Easy orbital and density analysis

Battery Discharge Voltages



www.scm.com/discharge-voltages-tutorial

Li-Ion Diffusion Coefficients



www.scm.com/diffusion-coefficients-tutorial

Spectroscopy

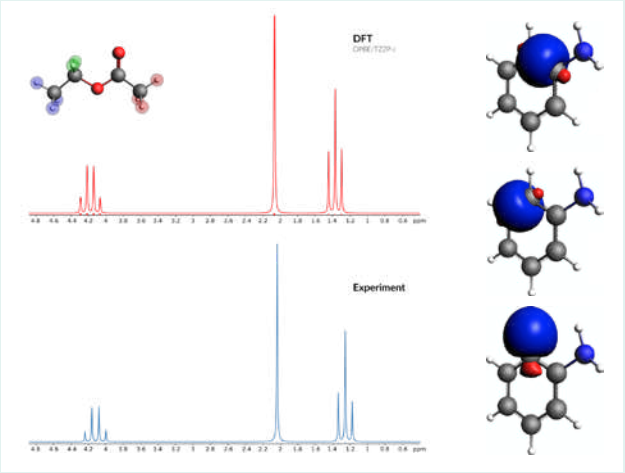
www.scm.com/applications/spectroscopy/

ADF is trusted for predicting magnetic, electric, optical and vibrational spectra, from NMR to X-ray. Relativistic Hamiltonians and Slater orbitals yield accurate spectroscopic property predictions with DFT.
Very well suited for transition metals and heavy elements.
Predict luminescence in d- and f-elements (e.g. lanthanides) with Ligand field DFT (LFDFT).

Selected available spectroscopic properties

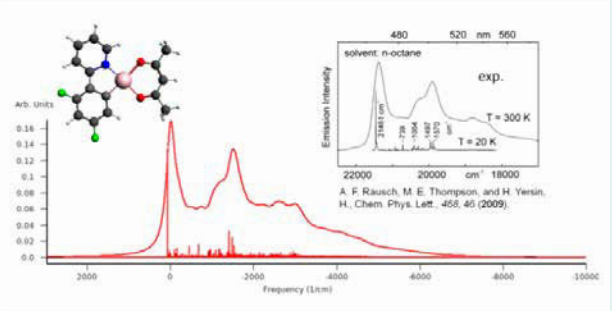
- UV-Vis: Fast and accurate TDDFT
- X-ray absorption: e.g. NEXAFS
- Various non-linear properties: e.g. TPA
- Many more: ESR, IR, VCD, CD, MCD, Mössbauer,...

Spin-spin coupling constants and NBO analysis



www.scm.com/nmr-tutorials

Franck-Condon Factors



www.scm.com/oled-tutorial-vibrational-progression

Polymers

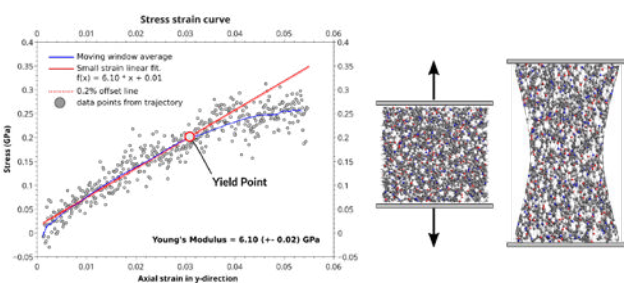
www.scm.com/applications/polymers/

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

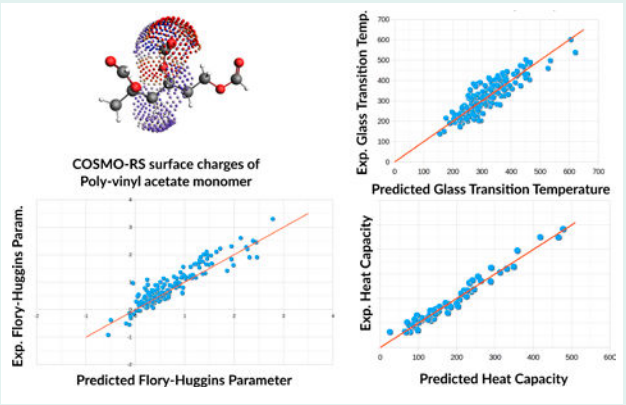
How will AMS modeling help you?

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

Mechanical Properties

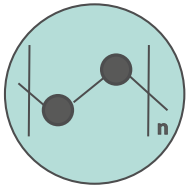


Flory-Huggins Parameters, Glass-transition Temperatures and more from COSMO-RS/UNIFAC



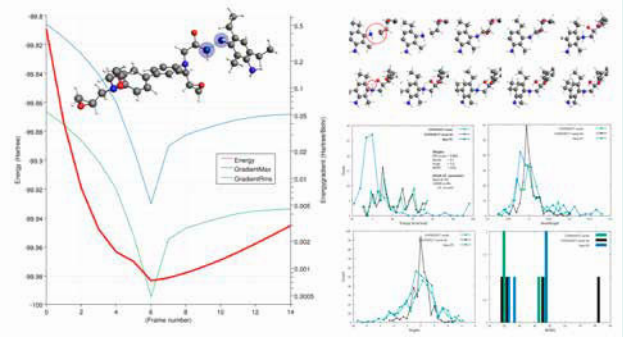
www.scm.com/cosmo-rs-polymers

Example workflow: Epoxide mechanical properties



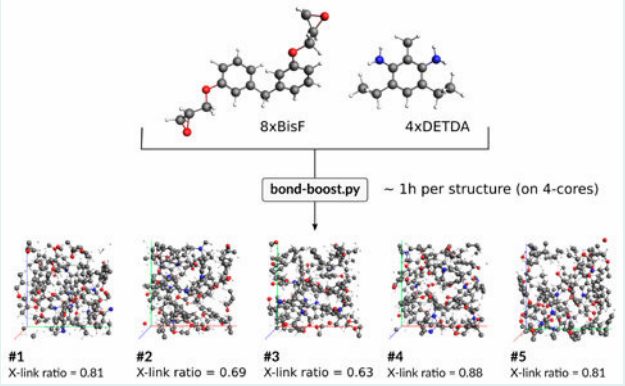
www.scm.com/applications/polymers/

STEP 1 — ADF DFTB GUI



- Study reaction profiles with DFT(B)
- Generate Training data
- Fit new ReaxFF Force Field

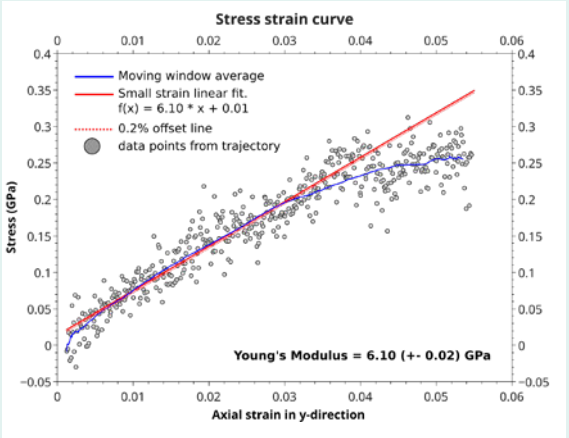
STEP 2 — ReaxFF PLAMS GUI

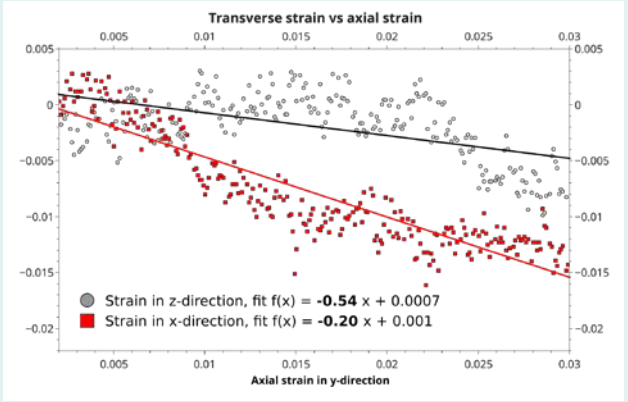


- Accelerate cross-linking reaction (“curing”)

STEP 3 — ReaxFF PLAMS GUI

Results: Young’s Modulus, Yield Points, Poisson’s Ratio,...





www.scm.com/epoxide-modeling

Oil & Gas

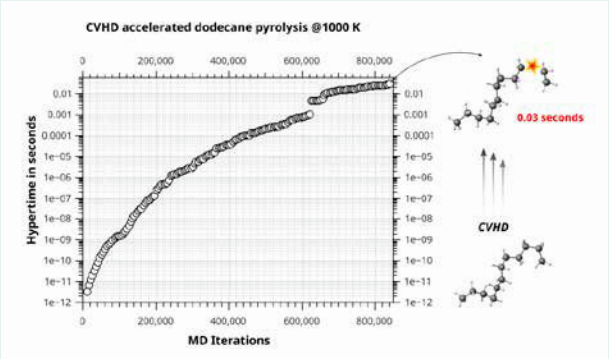
www.scm.com/applications/oil-and-gas/

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

How will AMS modeling help you?

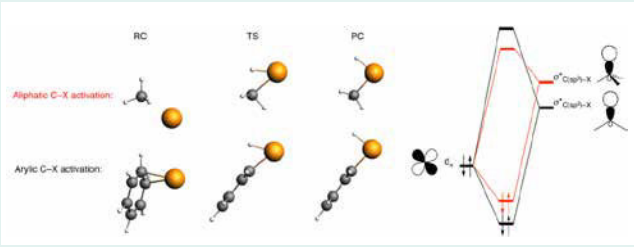
- Analyze combustion reaction networks / kinetics
- Accelerate reaction dynamics
- Bonding Analysis: Activation strain model for rational catalyst design
- Optimize solvents for extraction and other chemical processes

Combustion/Pyrolysis at realistic Temperatures



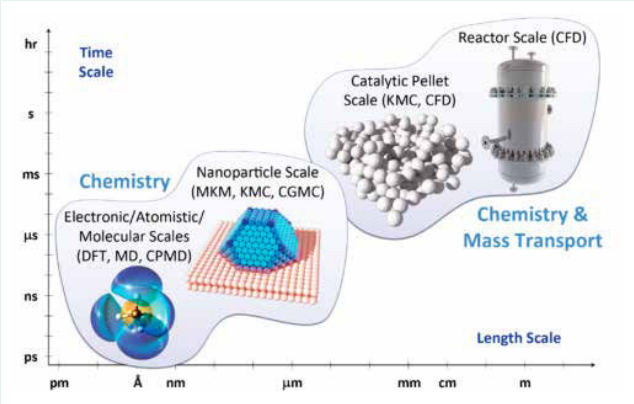
www.scm.com/cvhd-pyrolisis-tutorial

Facile C-X bond activation explained with relativistic DFT



www.scm.com/c-x-bond-activation-paper

Development of a multi-scale materials modeling platform to optimize chemical reactors



www.scm.com/multiscale

Nanotechnology

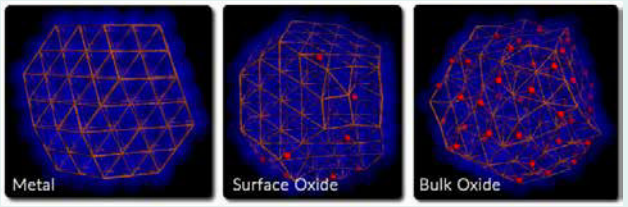
www.scm.com/applications/nanotechnology/

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

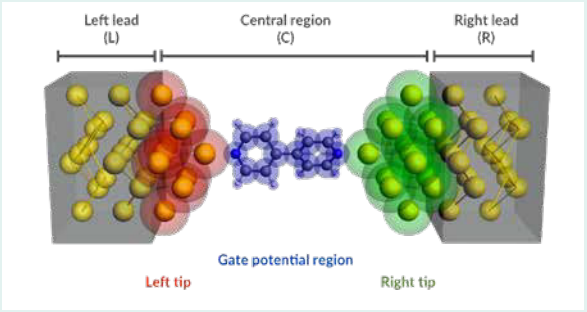
- Accurate relativistic effects with ZORA
- Frozen density embedding for environment effects and large systems
- Fast TD-DFT with Model Potentials (SAOP, LB) and many spectroscopic properties
- 1000s of atoms with (TD)DFTB and Millions of atoms with ReaxFF

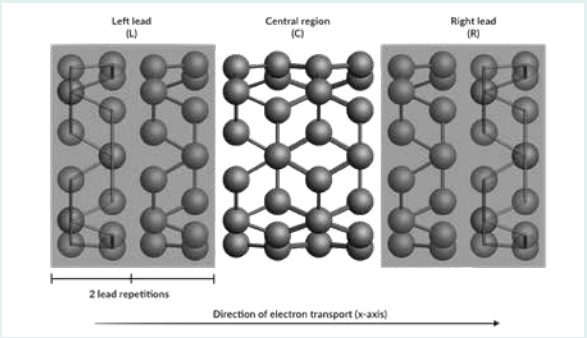
Pd-Catalysts oxidation under operating conditions



www.scm.com/gcmc-catalyst-tutorial

Charge transport with non-equlibrium Greens functions





www.scm.com/negf-tutorials

Life Sciences

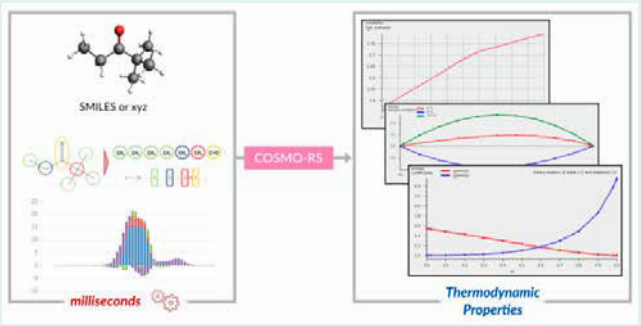
www.scm.com/applications/pharma/

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

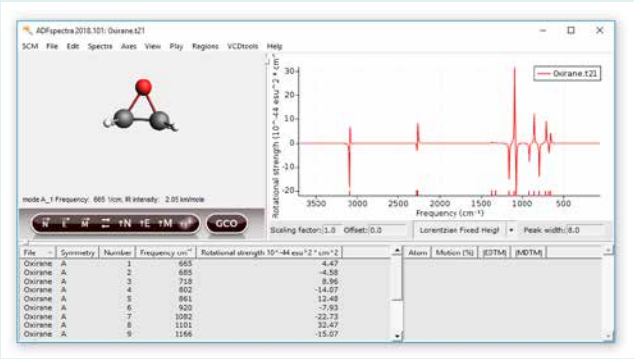
- Solubilities, logP, pKa, VLE, etc. based on DFT + thermodynamics
- Solvent optimization, e.g. for liquid-liquid extraction or recrystallization
- Accurate NMR predictions and analysis
- VCD analysis tools
- Accurate energies of organic crystals with DFTB+D

Ultrafast estimation of thermodynamics for screening



www.scm.com/cosmo-rs-screening-tutorial

Absolute configurations: Predict and analyze VCD



www.scm.com/vcd-tools-tutorial

Inorganic Chemistry

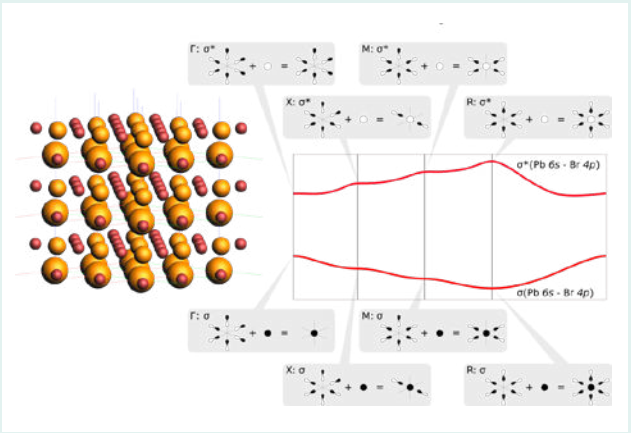
www.scm.com/applications/inorganic-chemistry

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

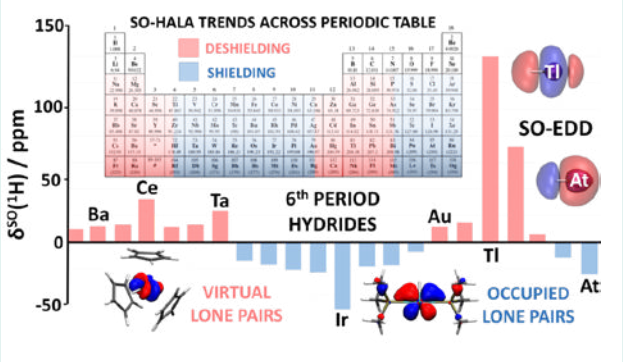
- From NMR to X-ray: Many spectroscopic properties
- Unique chemical bonding analysis
- Scalar-relativistic and spin-orbit coupling
- Slater-type all-electron, basis sets for all elements
- Robust SCF convergence methods

Bonding in metal halide perovskite explained



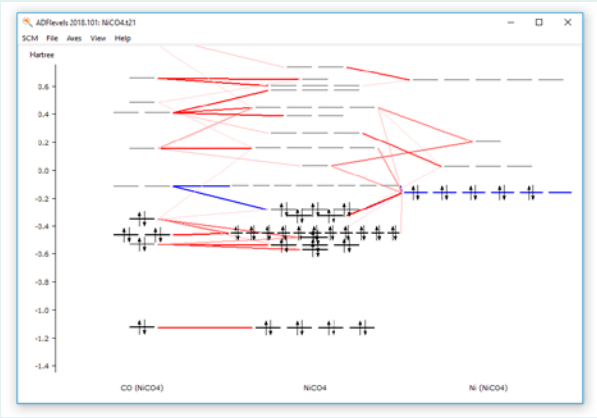
www.scm.com/band-coop-tutorial

NMR SO-HALA effect explained across the periodic table



www.scm.com/so-hala-nmr

Easy visualization of results



AMS Engines

www.scm.com/doc/AMS/Engines.html

ADF Amsterdam Density Functional is a powerful DFT program, trusted for understanding and predicting structure, reactivity, and spectra of molecules.

BAND is an atomic-orbital based DFT program for systems of any periodicity, including nanotubes and surfaces.
Accurate for heavy elements, spectroscopy, orbital and density analysis.

DFTB is a fast approximation to DFT, enabling larger systems or screening of larger data sets.
DFTB includes Grimme's new GFN1-xTB method for accurate structures and vibrational frequencies of all elements (Z=1-86).

MOPAC is a semi-empirical program for quick modeling of large systems of any periodicity.

ReaxFF is a reactive force field approach from the work of Prof. Adri van Duin and coworkers.

COSMO-RS the COnductor like Screening MOdel for Realistic Solvents is a program for instantaneous thermodynamic predictions of (mixed) fluids.

External run external programs as AMS engine: Combine the functionality in the AMS driver with any molecular modeling program.

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