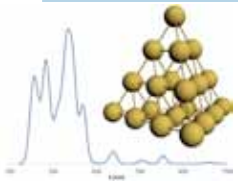
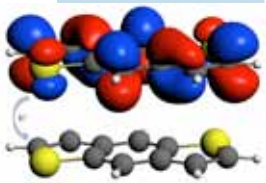
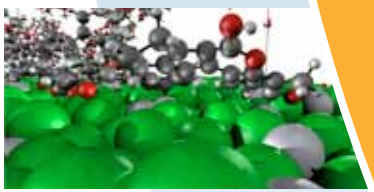
Scientific Computing & Modelling







Supported by

Seascape

www.seascapelearning.com

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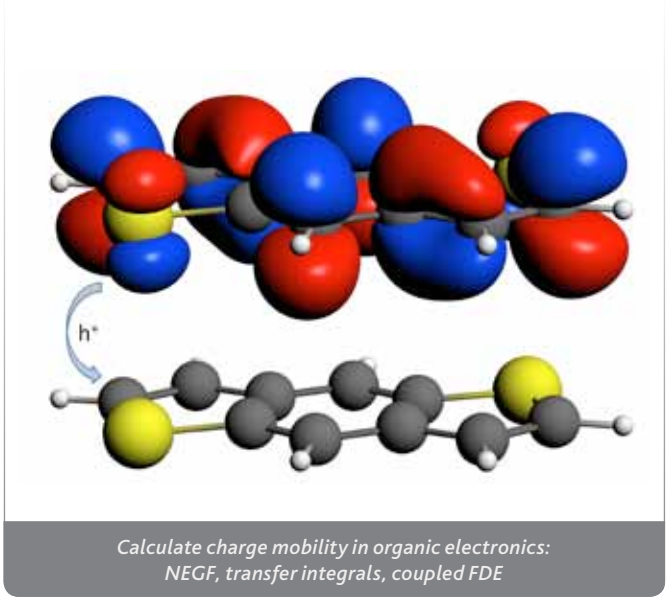


Calculate charge mobility in organic electronics: NEGF, transfer integrals, coupled FDE

Key benefits

One-stop modeling shop

Excellent software suite for tackling the most challenging problems in materials science and chemistry. Easy set up and analysis with GUI.

Fast computational toolbox

Working with hardware vendors, we optimize our codes for desktop computers and parallel supercomputers. Latest algorithms.

Heavy elements & spectroscopy

High-quality all-electron Slater basis sets for all elements. Accurate relativistic treatment. Many spectroscopic properties, from NMR to X-ray.

Understand chemical bonding

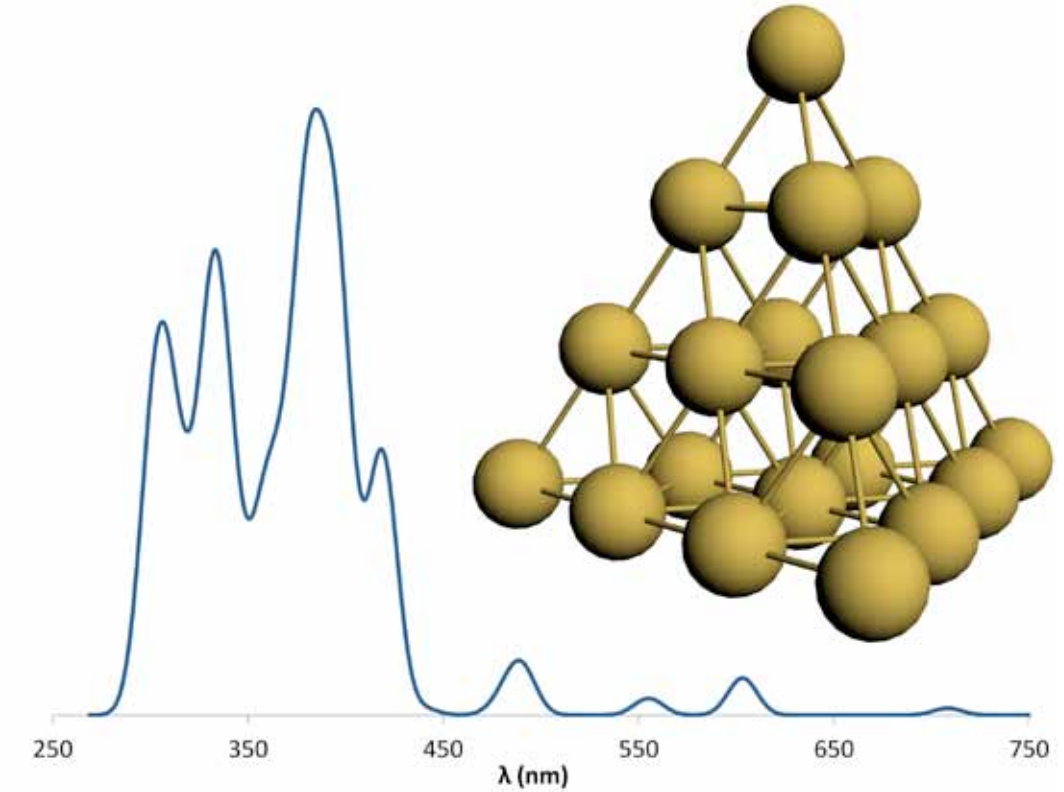
Unique insight in chemical bonds with many chemical analysis tools. Balanced charge decomposition schemes. Various density analysis tools.

Hassle-free installation, free trial

With parallel binaries for all popular platforms, the entire ADF suite installs out of the box. Try our powerful modeling tools: *scm.com/trial*

Discuss your science with experts

With decades of experience, our expert support team (PhDs in chemistry & physics) will help you with any queries that may arise.



Au_{20} UV/VIS spectrum, calculated within 20 minutes on a desktop PC

Capabilities

Organic electronics, unique features

- SOC-TDDFT: phosphorescence lifetimes for OLEDs
- Charge mobility calculations for OFETs, organic semi-conductors
- Accurate spectra of dyes, energy flows in dye-sensitized solar cells

scm.com/OrganicElectronics

Accurate spectroscopy

From EPR to XANES, we offer a very broad range of spectroscopy. ADF is particularly recommended by users for its excellent capabilities for NMR and optical spectra.

scm.com/Spectroscopy

Advanced environment/solvation options

- 3D-RISM: solvation calculation with averaged solvent structure
- QM/QM: frozen-density embedding, QUILD
- DRF, SCRF: polarizable environments for MD and QM/MM
- DIM/QM: coupled TDDFT + atomistic electrodynamics for SERS, plasmon-exciton hybridization

scm.com/Solvation

Understand chemical bonds

ADF is used by those who truly want to understand chemical bonding. Tools like energy decomposition, NBO, ETS-NOCV, NCI, AIM, bond orders, Hirshfeld give unique insight.

scm.com/ChemicalAnalysis

Structure & reactivity

Find TSs with NEB or Transition State Reaction Coordinate (TSRC). Find shallow minima with fine integration and delocalized coordinates. Rationally design catalysts with the activation strain model.

scm.com/StructureAndReactivity

True 1D and 2D systems, compare periodic with cluster

Model polymers and surfaces without artificial repetition in other dimensions. Compare bulk and cluster by using exact same set up. Include surface solvation and electric fields. All-electron basis sets for all elements.

scm.com/PeriodicDFT

Fast approximate DFT for large molecules

Density functional-based tight binding uses pair-wise parameters for fast calculations, enabling you to study systems up to thousands of atoms. Molecules, polymers, surfaces, bulk.

scm.com/DFTB

Atomistic modeling of large, reactive systems

ReaxFF was designed to tackle engineering challenges at the atomistic level. Model the reactive dynamics of complex, inhomogeneous systems up to 100,000s of atoms.

scm.com/ReaxFF

Solubilities, partition coefficients (log P), pK_a

Predict many properties of pure fluids, mixtures and solutions instantaneously with COSMO-RS. An easily expandable database of 1892 compounds, allows you to prescreen solvent combinations with the right properties for drug solubility and contamination partitioning.

scm.com/COSMO-RS

Robust, parallel, efficient

We work with all major hardware vendors to scale up to 100s of CPUs, and to exploit GPUs. Efficient algorithms for SCF and geometry optimization are continuously being implemented.

scm.com/Parallel

Set up, run, and analyze all your modeling jobs effortlessly

Get to work quickly with our step-by-step tutorial and videos!
A fully integrated graphical user interface makes it easy to switch between different compute engines and visualization tools. A large database of compounds and import tools makes set up a breeze. Advanced scripting tools to set up and analyze many jobs all at once.

scm.com/GUI

ADF: Amsterdam Density Functional

Molecular research questions? ADF is the answer!

Our flagship program ADF has a 40-year track-record in handling the most difficult problems in all areas of chemistry and materials science. Accurate, fast, and robust software to study intricate bonding and spectroscopy properties from simple to exotic compounds.

Ever-expanding functionality

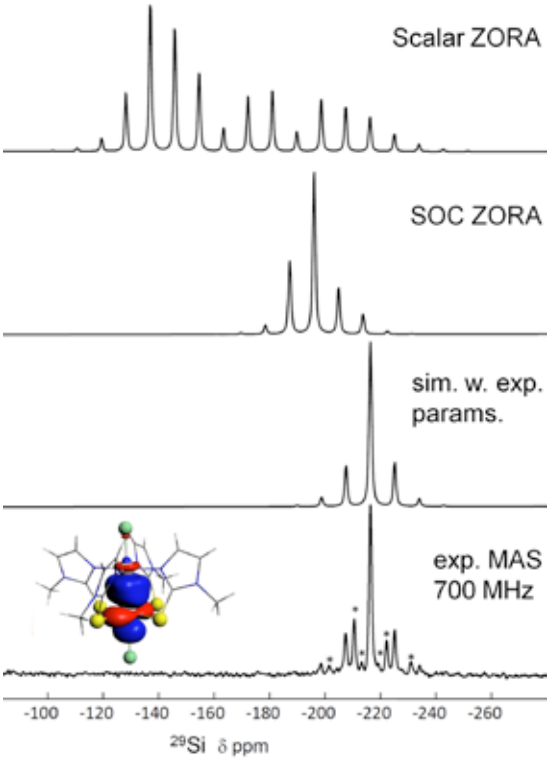
With our partners in industry and academia we keep implementing the latest xc functionals and capabilities to ensure ADF can answer your research questions also in the future.

Strong points

- fast and well-parallelized
- spectroscopy
- transition metals, heavy atoms
- user-friendly set-up & support
- truly understand chemistry

Selected unique features

- spin-orbit coupling TDDFT
- charge transfer integrals, Green's functions
- scrutinize chemical bonding interactions
- Slaters: correct nuclear cusp (NMR, EPR)
- environment: DIM/QM, 3D-RISM, FDE
- energy decomposition, fragments



Relativity: only spin-orbit coupling gets ^{29}Si NMR spectral peak shape right. Angew. Chem. Int. Ed. 50, 255 (2011)

BAND: Periodic DFT

What can BAND do that your plane wave code cannot?

- perfect companion to ADF: cluster & periodic with same settings
- treat all electrons
- treat surfaces as true 2D, polymers as true 1D
- treat relativistic effects properly
- include homogeneous electric fields
- include continuum solvation (COSMO)
- make life easy: build and visualize with GUI
- calculate many spectra, orbitals & density properties

Selected BAND features

- **spectra**: NMR, EPR (g & A tensors), EFG, Q-tensor, EELS
- **analysis**: (P)DOS, band structures, COOP, AIM, ELF, fragments
- lattice optimization, phonons
- metal dielectric functions: TDCDFT
- latest functionals: Grimme D3(BJ) dispersion, Truhlar mGGAs
- specialized band gap functionals: GLLB-sc, TB-mBJ, GGA+U

DFTB, MOPAC2012

Study really big systems at the quantum level

Our advanced multi-level schemes in ADF are not suitable for partitioning your large molecule? Periodic systems with very large unit cells?

Stewart's semi-empirical MOPAC2012 and our density-functional based tight binding (DFTB) modules could bring the quantum precision you need to study these systems.

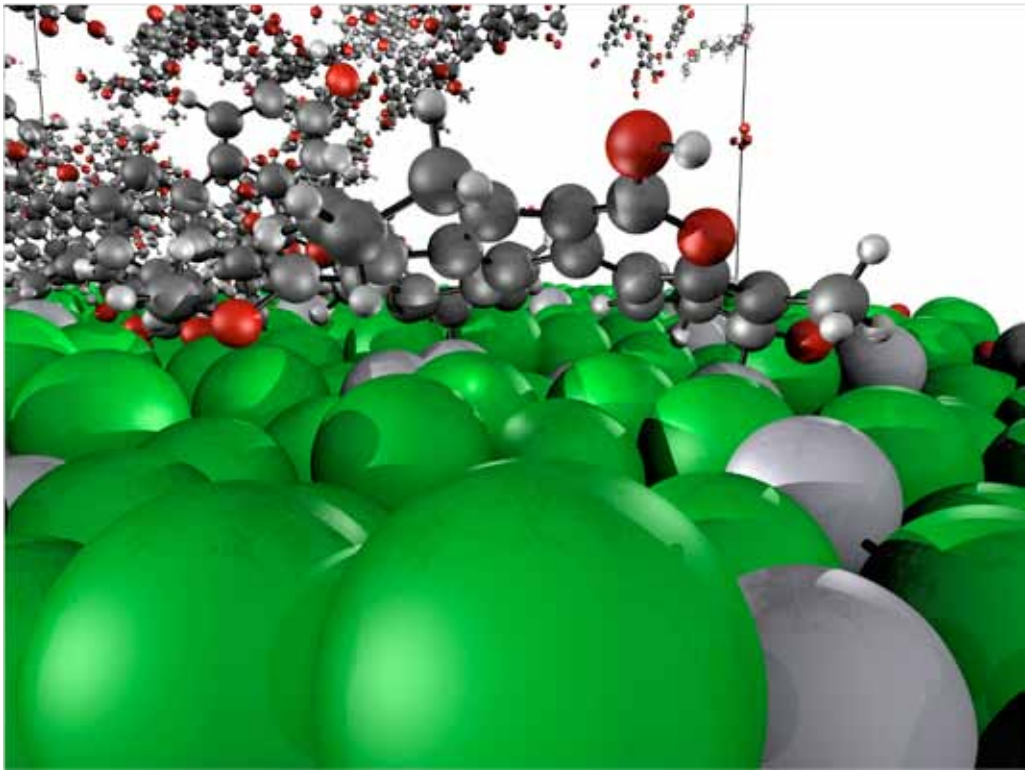
Quick insight, pre-screening or pre-optimization

With parameters for almost the entire periodic table, MOPAC2012 is a great tool for pre-optimization and pre-screening of conformers before you dive in to more accurate DFT calculations. We and our academic partners are determined to make DFTB parameters for most nuclei, enabling you to get insight in the dynamic behavior of various nano-sized systems.

MOPAC2012	H-Bi, Sparkles: lanthanides, molecules, 1D, 2D, 3D, PM7, PM6, and more.
DFTB	SCC, DFTB3, molecular dynamics, molecules, 1D, 2D, 3D, parallelized, properties

QUOTE

"What I really like about ADF? The programs were clearly written by chemists for dealing with real chemical problems. A great suite of programs!"
***Prof. Roald Hoffmann** - Nobel Laureate chemistry*



ReaxFF simulation of MoNi-catalyzed coal combustion (M. Russo, A. van Duin)

ReaxFF

Study chemical reactions in really, really large systems

- Model 100,000s of atoms with the reactive MD module ReaxFF
- Easy building of complex homogeneous mixtures and surface-liquid interfaces alike with the GUI
- Visualize and analyze the changing molecular composition on the fly

ReaxFF parameters

We collaborate with Prof. van Duin and others to include the latest optimized force field parameters. Working on automated procedures to construct your own force fields.

We keep on top of algorithmic developments to increase accuracy and speed.

Dynamics

Define different temperature regimes, start with non-reactive iterations. NVT, NVP, NVE. Accelerated dynamics available via interface. Visualize trajectories.

Application areas

- nanoscience
- material science
- biochemistry
- combustion chemistry
- polymer chemistry
- catalysis

COSMO-RS

Instantaneous prediction of

- solubilities
- partition coefficients
- pK_a values
- vapor-liquid, liquid-liquid equilibria (VLE/LLE)

... and much more

- activity coefficients, solvation free energies
- Henry's law constants
- partial/total vapor pressures
- boiling points of solvents and mixtures
- excess energies G^E, H^E and TS^E
- azeotropes, miscibility gaps

COnductor-like Screening MOdel for Realistic Solvents

Thermodynamic properties calculated with quantummechanical based COSMO-RS have predictive power outside the parameterization set, as opposed to empirical models (UNIFAC).

Extensive database of compounds, easy to expand

Almost 1900 molecule are included in a database. Predict the solubility or solvent partitioning for your own drug? Simply add your own substances to our database with a fixed ADF recipe!

QUOTE

"The GUI of ADF is one of the best builders I have ever used, the possibility to create everything from simple ADF calculations to complex QM/MM setups to band structure calculations make it very appealing. Constructing metal complexes has never been so easy."
***Dr. Michael Patzschke** - University of Helsinki*

Fully integrated GUI: Build, Run, Analyze!

Build

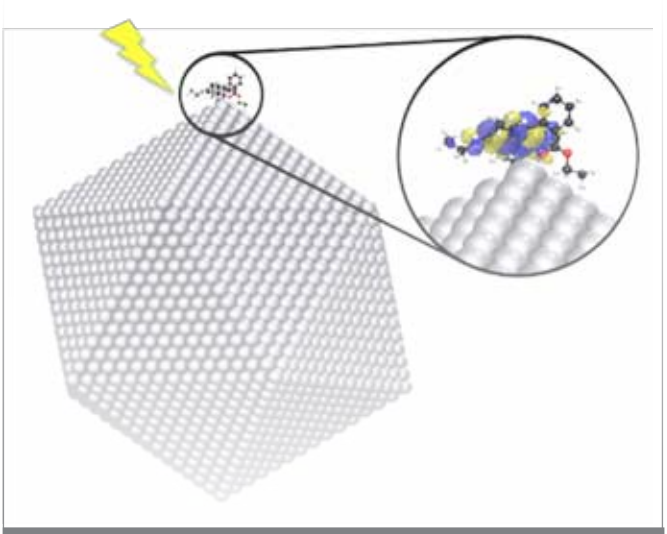
- import cif, xyz, smiles
- large database of structures
- slice surfaces, create supercells
- switch from molecular to periodic
- build complex mixtures with Packmol

Run

- Windows, Mac, Linux
- cross-platform compatible, remote queues
- easy switching from DFT to DFTB or MD and back

Analyze

- quick visualization of MOs, densities, properties
- (partial) DOS, band structures, many spectra
- movies of vibrations, optimization, MD trajectories



DIM/QM: excited state QM/MM for molecules on nanoparticles (L. Jensen)

Background

History
ADF originates from the academic work of Prof. Baerends (VU Amsterdam) and Prof. Ziegler (University of Calgary). In 1995, the company Scientific Computing & Modelling NV was founded in Amsterdam, and as of 2013 SCM employs 14 people, mostly highly trained (PhDs) academics. With 3 successful EU projects we continue to expand with several job openings and development plans.

Academic network: cutting-edge tools
Staying close to the academic community is paramount to us. It keeps us on top of the latest developments in order to satisfy the most pressing modeling demands of today and the future.

Academic developers are happy to see the burdens of debugging, porting, testing and documenting taken off their hands by our experienced software developers.

Documentation, support
Extensive documentation and step-by-step tutorials on our web quickly help you on your way to set up calculations. The GUI has a useful search function for features and molecules. Expert support (support@scm.com) and a mailing list are available for all users.

Platform compatibility
The binaries work out of the box on the most popular (Windows, Mac, Linux) platforms as well as for popular HPC architectures (Cray, SGI, AIX, Altix, ...). We offer help with compiling and optimizing on non-standard systems on a no-cure, no-pay basis.

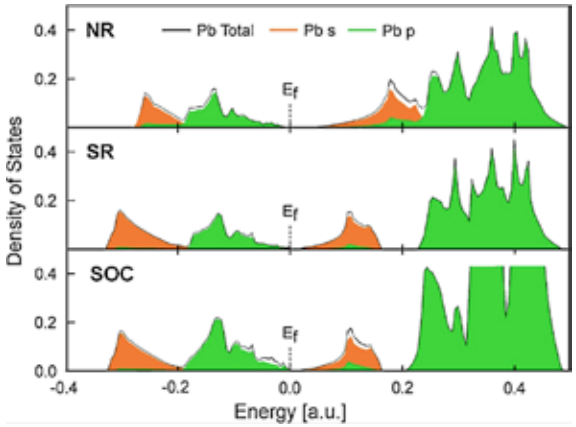
Licensing, pricing
Licenses are multi-platform and host-locked or floating. We can tailor the license to your specific situation and modeling requirements. Pricing depends on which modules you want, the type of institution, number of cores and number of years. We offer regional discounts and teaching-only discounts.

www.scm.com/Sales lists academic prices; you may also request a quote from there.

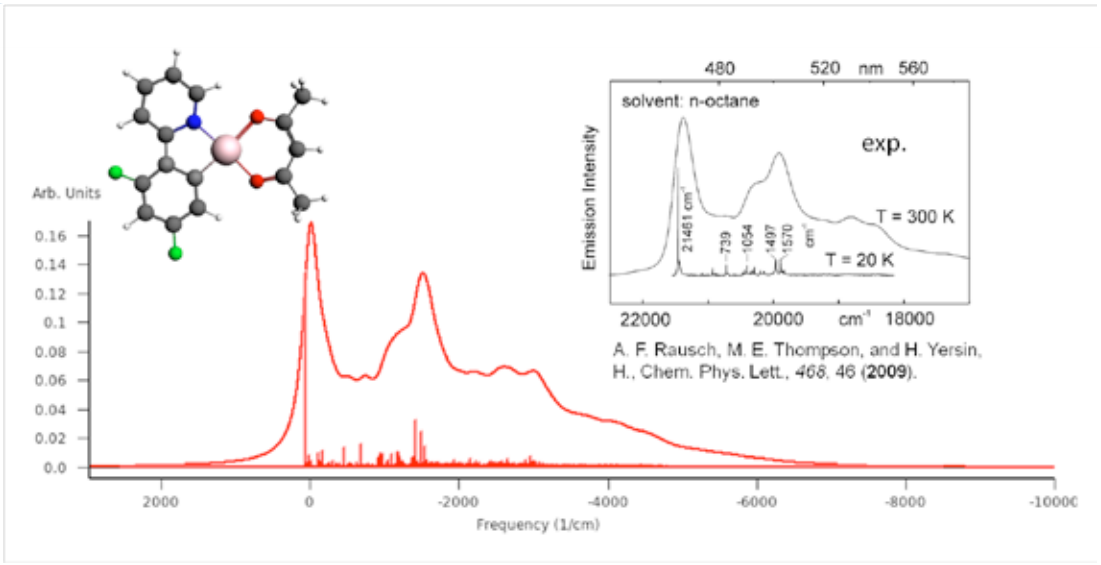
Consultancy & Contract research
Contact us at info@scm.com if you are interested in consultancy options or contract research for your custom modeling needs. Upon request we may also implement specific features.

QUOTE

"I was very impressed by the quality of the support and their efficiency"
***Romaric David** - head HPC Strasbourg University*



Relativity increases lead acid battery voltage from 2.4V to 12V!
Phys. Rev. Lett. 106, 018301 (2011)



Vibrational fine structure of $T_1 \rightarrow S_0$ emission from OLED emitter in good agreement with experiment (Mr. Kento Mori, Ryoka Inc.)

Feature list

ADF: molecular DFT

Structure and Reactivity
- optimization (ground and excited states)
- transition states (TS reaction coordinate, EF, NEB), IRC, LT
- (analytical) frequencies, initial Hessian estimates, constraints and restraints
- Cartesian, internal, delocalized coordinates

Model Hamiltonians
- relativistic effects (ZORA, spin-orbit coupling)
- modern xc: LDA, GGA, (range separated) hybrid-GGA, meta-GGA, meta-hybrid-GGA
- dispersion corrections: D3, D3-BJ, dDsC
- potential-only: SAOP, GRAC, LB94, OEP
- energy-only: more (hybrid) (meta-)GGAs
- solvents, environments: COSMO, QM/MM, DRF, FDE, SCRF, 3D-RISM, QUILD, DIM/QM
- electric field, point charges
- finite nuclei

Electronic transport
- transfer integrals
- non-self-consistent Green's function, wide-band limit
- coupled FDE

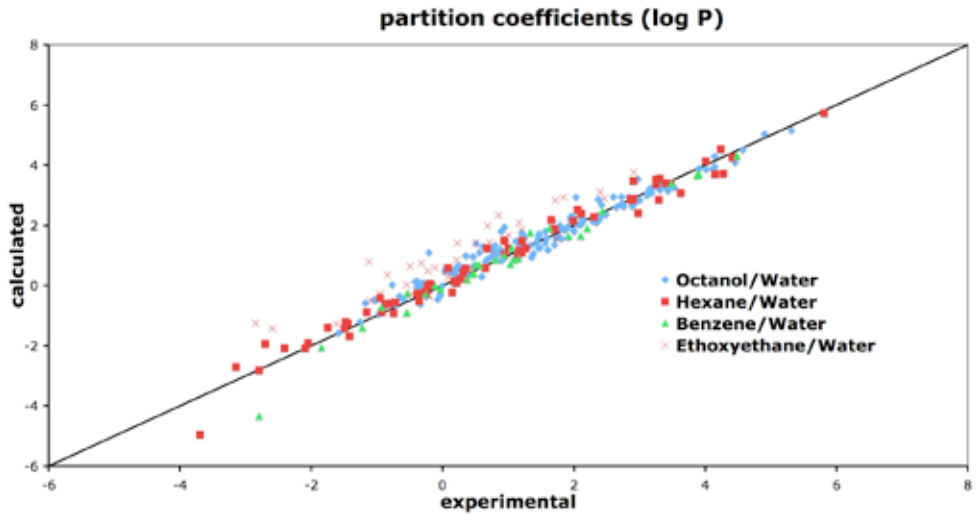
Spectroscopic properties
- IR, (resonance) Raman, MBH, VCD, VROA, Franck-Condon factors
- (vibrationally resolved) UV/Vis spectra, X-ray, core excitations, state selection
- CD, ORD, magnetizabilities, MCD, Verdet constants, Faraday terms
- (hyper-)polarizabilities, dispersion coefficients, lifetime effects
- NMR chemical shifts, spin-spin couplings
- ESR (EPR): g-tensor, A-tensor, Q-tensor, D-tensor (ZFS)
- Nuclear quadrupole interaction (EFG), Mössbauer, NRVS

Analysis
- molecule from fragments, symmetry
- bond energy analysis, ETS-NOCV
- Mulliken, Voronoi, and Hirshfeld charges, bond orders, NBO6, NCI, SEDD, AIM, ELF, (partial) DOS

Accuracy and Efficiency
- High-quality Slater basis sets Z = 1 to 118, all-electron, frozen core, SZ to QZ4P
- parallelized, linear scaling, distance cut-offs, density fit
- LISTi, ADIIS, EDIIS, ARH, and spin-flip for flexible and robust SCF convergence

QUOTE

"The ADF program suite has very useful features that make it stand out in comparison to other codes. Clusters and extended systems can be directly compared, and switching relativistic effects on and off gives unique insight."
***Dr. Michael Patzschke** - University of Helsinki*



Solvent/water partition coefficients (log P): experimental vs COSMO-RS

BAND: periodic DFT

- bulk crystals, polymers, surfaces
- geometry optimization (including lattice), transition state search, frequencies
- XC: LDA, GGA, meta-GGA, dispersion corrections (D3, D3-BJ), GGA+U, HTBS, GLLB-sc, TB-mBJ
- relativistic effects with ZORA and spin-orbit coupling: SCF and forces
- finite nucleus approximation
- COSMO solvation model for surfaces, static homogeneous electric fields
- TDDFT: frequency-dependent dielectric functions, EELS, SO effects, Vignale-Kohn functional
- DOS (total, partial, local), Mulliken population analysis, form factors, AIM, ELF
- STM images, smooth band structures, phonon dispersion curves, Fermi surfaces
- effective mass tensors
- bond energy analysis (fragment approach)
- NMR chemical shifts, shielding tensors
- electric field gradient (NQCC)
- ESR (EPR): A-tensor, g-tensor
- parallel, linear scaling techniques
- numerical orbitals and high-quality all-electron Slater orbitals for all elements, SZ to QZ4P

DFTB

- 2nd, 3rd order self-consistent charges (SCC, DFTB3), dispersion corrections
- minima and TS optimization molecules and periodic (1D, 2D, 3D) systems
- molecular dynamics with Velocity Verlet, Berendsen and scaling thermostats
- phonons, DOS, band structure

MOPAC2012

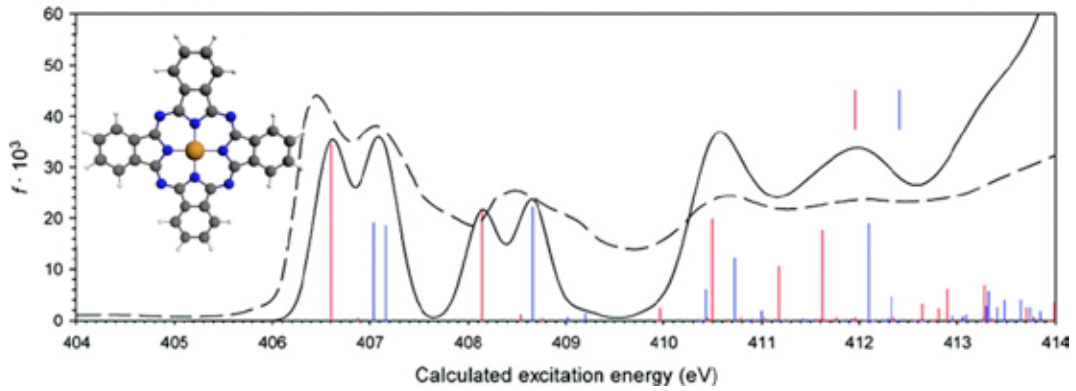
- molecules and periodic systems (1D, 2D, 3D)
- minima and TSs, COSMO solvation
- Sparkle for lanthanides
- MOZYME: linear-scaling SCF for large systems
- PM7, PM7-TS, MNDO, AM1, PM3, PM6, PM6-DH+, PM6-H2

ReaxFF

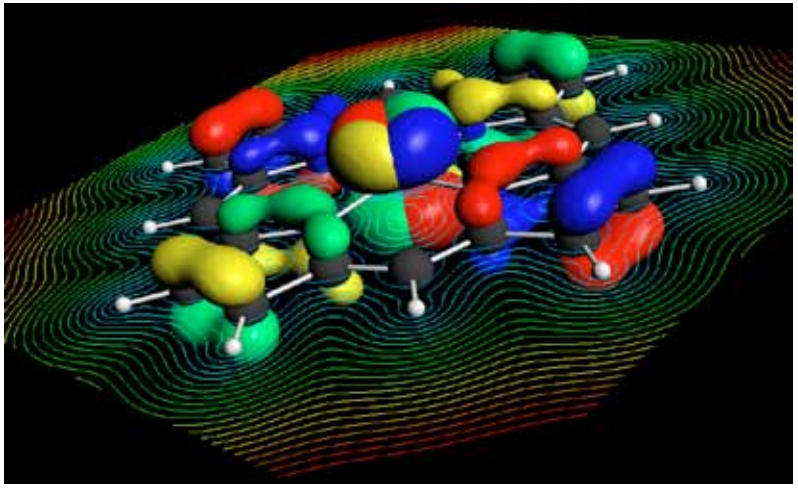
- parallelized molecular dynamics and minimizations with reactive force fields
- analyze changing composition (reactants, intermediates, products) during MD run
- Berendsen thermostat; NVT, NPT or NVE ensembles; constrained dynamics
- easy set up of complex mixtures and solid-liquid interfaces in 3D box with Packmol
- define different temperature regimes, pressure constraints, bond constraints
- up to 100.000s of atoms

COSMO-RS

- predict properties of solutions and liquids with COSMO-RS or COSMO-SAC
- solubilities, partition coefficients (log P), activity coefficients, solvation free energies, pK_a
- VLE (LLE) diagrams, boiling points, flash points, composition lines, miscibility gaps
- database of almost 1900 molecules



NEXAFS Spectrum of Metal Phthalocyanines with DFT-TS, J. Phys. Chem. A, 116, 2285 (2012)



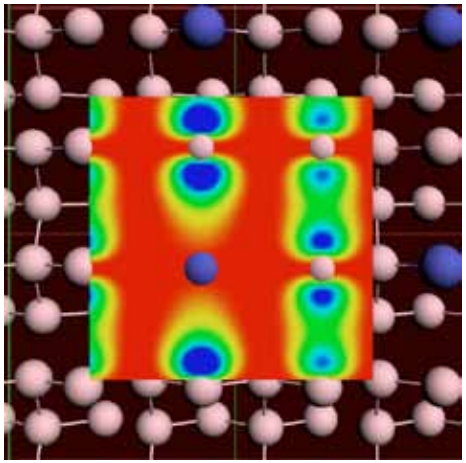
Quick and easy visualization of orbitals, contour plots, and much more

Integrated GUI

- set up, run and analyze (complex) jobs for all programs
- queue and monitor jobs on different machines
- search: panels, documentation, database
- draw molecules or import (extensive database, .xyz, .pdb, .cif, SMILES)
- pre-optimization with UFF, MOPAC, or DFTB
- easy set up of complex mixtures and solid-liquid interfaces in 3D box with Packmol
- seamless switching between all calculation and visualization modules
- 3D data fields for orbitals, densities, potentials and more
- field visualization via iso surfaces, cut planes or contour plots
- visualize DOS, IR, Raman, CD, MCD, VCD, optical spectra, and more
- electronic band structures, phonon dispersion curves with Brillouin Zone
- display (partial) Density-Of-States for ADF, BAND and DFTB
- draw orbital interaction diagrams (fragment approach)
- show vibrations, optimizations, and MD trajectories
- prepare multiple ADF calculations and compare results graphically and numerically
- monitor calculation progress, browse (live) output, for local and remote jobs

Tools

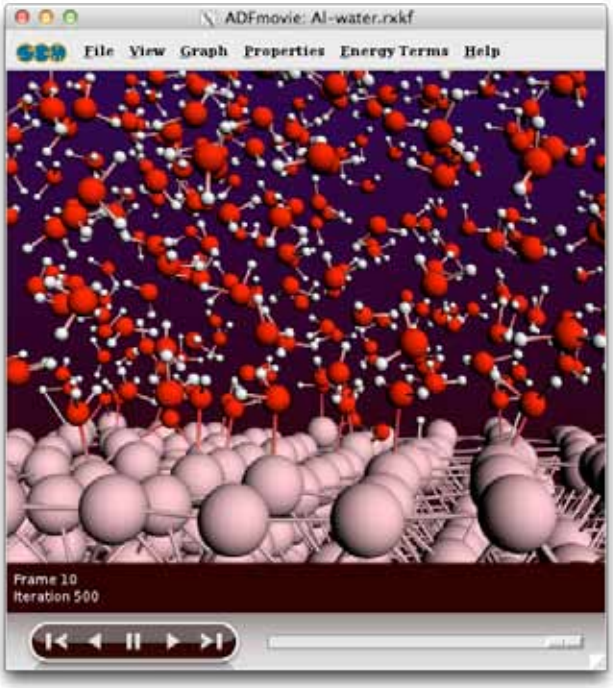
- QM/MM, QUILD: perform multi-layer calculations
- PyMD: advanced MD (multi-scale, adaptive, biased)
- scripting to prepare and report multiple complex jobs (PyADF)



Calculated STM image (LDOS) for PtGe(100)

QUOTE

"The support at SCM is truly top notch"
***Dr. Kwan Skinner** - Top 10 US chemical company*



Just a few clicks to set up and run a reactive MD run: water on Al surface

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