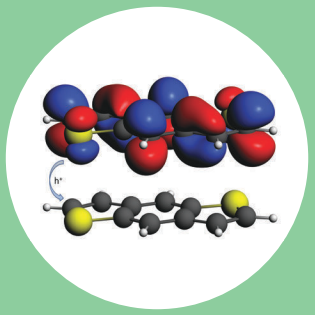
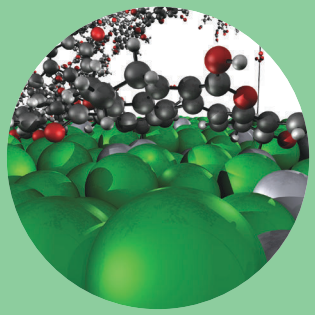
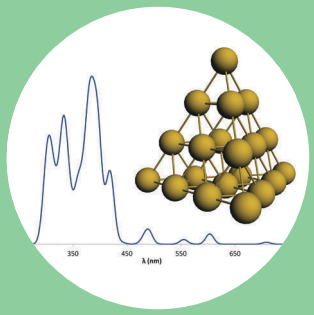
ADF Modeling Suite







SCM
Software for
Chemistry &
Materials

Making computational chemistry work for you

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ADF Modeling Suite

We aim to make computational chemistry work for you.

In collaboration with our partners we develop powerful tools ranging from DFT to fluid thermodynamics. The whole suite installs from a single file and the integrated graphical interface makes it easy to switch between molecules and periodic systems as well as from DFT to DFTB and ReaxFF. With parameterization and scripting tools, you can easily tailor our software to your needs.

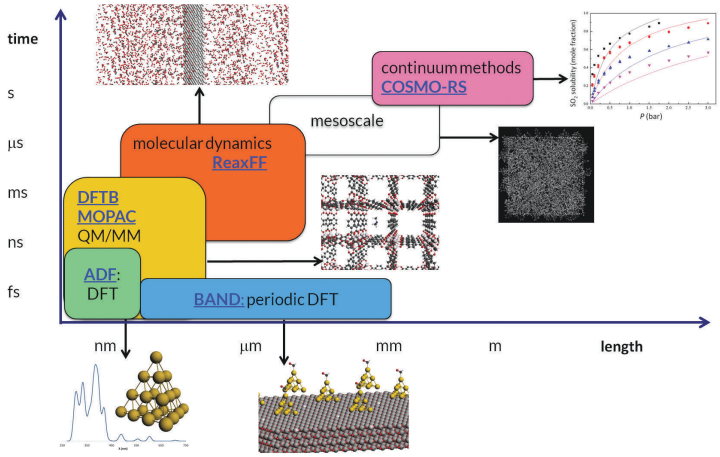
Strong points:

- use latest tools due to continuous development
- easy to use with one graphical interface for all modules
- get supported by the experts developing the code
- faster results with optimized binaries on common hardware

People behind the software

ADF originated in the 1970s from the theoretical chemistry group at the VU University in Amsterdam, resulting in the spin-off company Scientific Computing & Modelling in 1995. SCM, currently known as Software for Chemistry & Materials, has been steadily growing since then, with a team of about 15 passionate scientists. We maintain many collaborations and are proud to support our customers in academia, government and industry across the globe.

Our authors: www.scm.com/collaborations/our-authors/
Current EU projects: www.scm.com/collaborations/eu-projects/



Making computational chemistry work for you

Academic development
Ongoing academic collaborations empower scientists with the latest computational chemistry tools

Excellent GUI
Setting up, submitting and analyzing jobs is easy with the integrated graphical interface, running on Windows, Mac, and Linux

Expert support team
Excellent technical support directly from our developers with decades of experience - also during your trial

Parallel binaries
ADF runs in parallel out of the box on common hardware and can also be used in the cloud

Fully integrated graphical interface

The integrated graphical interface (GUI) works with all our codes on Mac, Windows and Linux, which makes it easy to set up and visualize different job types. The installation of the GUI and all computational engines is hassle-free from a single file.

Build

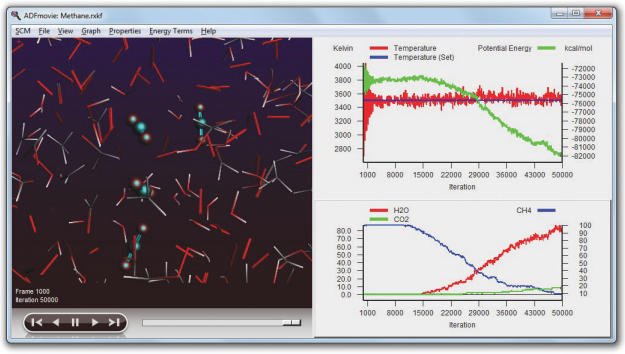
- import cif, xyz, smiles
- large database of structures, complex mixtures with Packmol
- slice surfaces, create supercells
- easy toggling between clusters and periodic systems

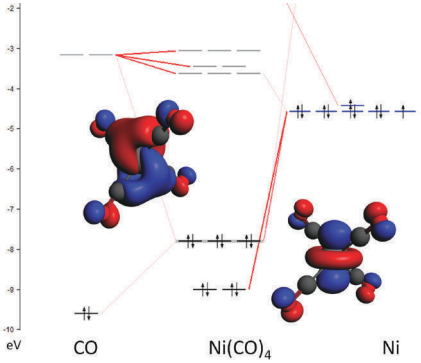
Run

- Windows, Mac, Linux
- cross-platform compatible, remote queues
- chained jobs, scripting, workflows

Analyze

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





ADF: molecular DFT

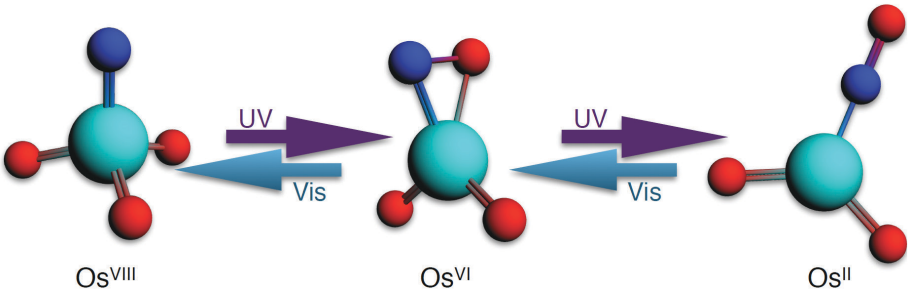
Our flagship program Amsterdam Density Functional (ADF) has a 40-year track record in handling the most difficult problems in chemistry and materials science. ADF is accurate, fast, and robust software to study chemical reactivity, intricate bonding and spectroscopic properties from simple to exotic compounds.

Strong points:

- accurate and efficient treatment of relativistic effects
- many spectroscopic properties from NMR to X-Ray
- insight in chemical bonding with detailed analysis
- advanced methods for including environment effects

Selected features:

- phosphorescence lifetimes with spin-orbit coupling TDDFT
- charge mobilities with transfer integrals and NEGF
- modern functionals, including meta-GGAs, long-range corrected hybrids, dispersion corrections
- Slater orbitals describe core electronic properties better (NMR, EPR)
- easy scripting for advanced jobs, workflows and high-throughput



Intramolecular 6-electron photo-redox reactions, Ang ew. Chem. Int. Ed. 54, 2072 (2015)

BAND: periodic DFT

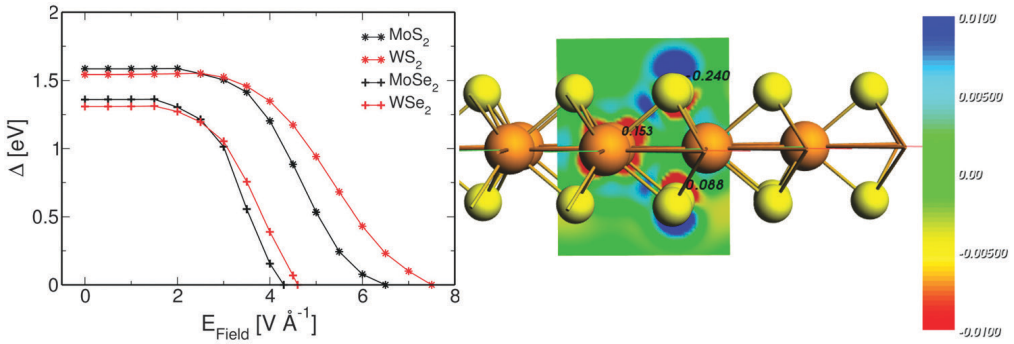
Our periodic DFT code BAND is a perfect companion to ADF, with the same basis sets and relativistic treatment. BAND is also strong in (core) electronic properties and analyzing orbitals and chemical bonds. It is particularly fast for low-dimensional and empty systems.

Strong points:

- easy to compare cluster and periodic with same basis sets
- spectroscopic properties, including core electrons (NMR, EPR, NEXAFS)
- real 1D and 2D: no artificial repetition in 3D
- all-electron basis sets for all elements: no pseudopotential approximation
- self-consistent spin-orbit coupling

Selected features:

- continuum solvation: COSMO, SM12
- homogeneous electric fields
- analysis tools: orbitals, pEDA, (p)DOS, QT-AIM, COOP, ELF
- modern functionals, including meta-GGAs, range-separated hybrids, dispersion corrections



Closing the band gap in 2D semiconductors, Phys. Chem. Chem. Phys. 16, 11251-11255 (2014).

DFTB, MOPAC: semi-empirical

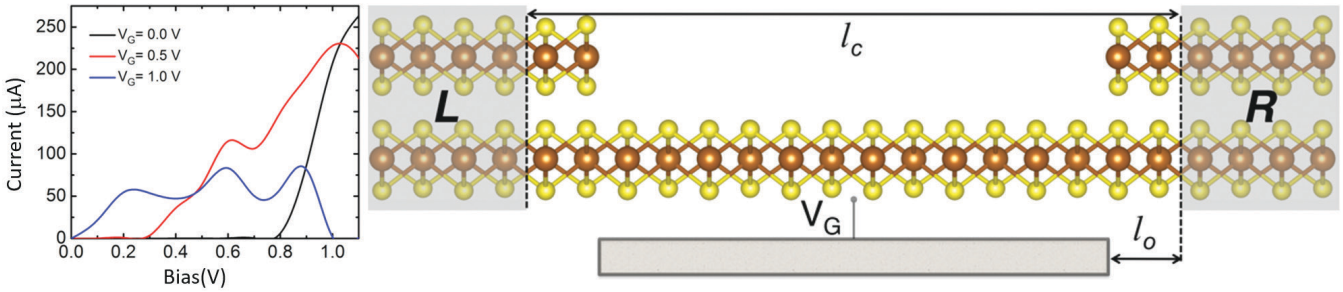
Our density-functional based tight binding (DFTB) and MOPAC are both fast codes which could bring the quantum precision you need to study large molecules or periodic systems. A good trade-off between speed and accuracy is achieved through a minimal basis and parameterization.

Strong points:

- quick pre-optimization, fast screening, and scriptable workflows
- molecules as well as proper 1D, 2D, and 3D periodicity
- most elements available for electronic DFTB and MOPAC
- easy incorporation in multi-layer models

Selected DFTB features:

- parameters: DFTB.org, Quasinano 2013 & 2015, dispersion corrections
- spectroscopy: IR, phonons, UV/VIS, Franck-Condon factors
- quantum transport with NEGF
- molecular dynamics
- orbital visualization



Logical junction from 2D PbS_2 only, Adv. Mater. 2016, 10.1002/adma.201504274

ReaxFF: reactive MD

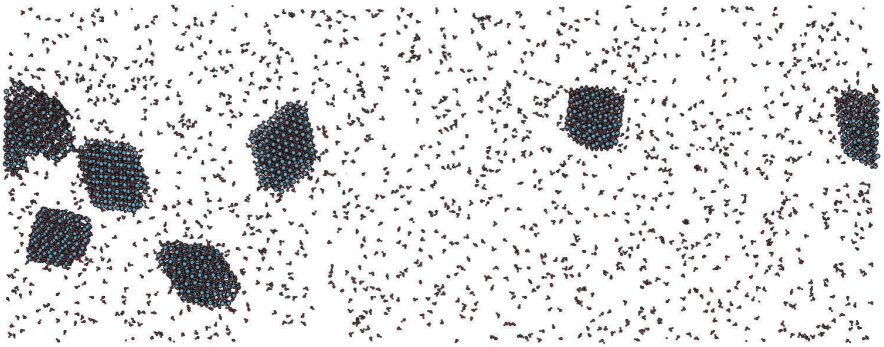
Study chemical reactions and molecular dynamics in large, complex systems with ReaxFF. We continue to improve usability and functionality in collaboration with Prof. van Duin and other partners. ReaxFF is applied in all areas of chemistry and materials science, most notably combustion, batteries, glasses, polymers, biochemistry, and catalysis.

Strong points:

- easy building and set up of complex simulations
- analyze and visualize changing composition on the fly
- automated reaction path detection
- many force fields included, (re)parameterize with MCFF optimizer

Selected ReaxFF features:

- optimization, non-reactive MD, reactive MD
- specify different T, V, and E regimes
- grand-canonical Monte Carlo: reactivity under equilibrium conditions
- force-biased Monte Carlo: accelerated reactive MD
- ACKS2: correct long-range charge behavior (batteries, enzymes)



Oriented attachment of TiO2 nanocrystals, Nano Lett. 14, 1836-1842 (2014)

COSMO-RS: fluid thermodynamics

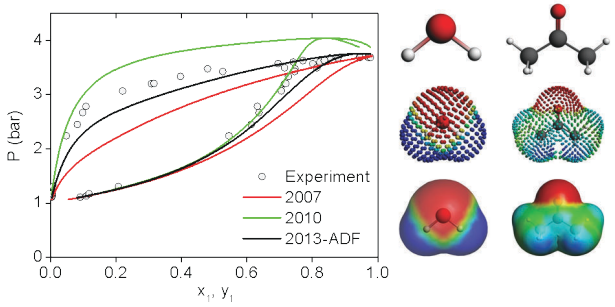
The COnductor-like Screening MOdel for Realistic Solvents calculates thermodynamic properties of fluids and solutions based on quantum mechanical data. Properties from COSMO-RS have predictive power outside the parameterization set, as opposed to empirical models (e.g. UNIFAC).

Strong points:

- predict many properties instantaneously (solubilities, logP, vapor-liquid equilibrium, ...)
- improved solvation energies and pKa values compared to COSMO
- quick screening with easy preparation and reporting scripts
- database of 1892 molecules, easy to expand with fixed ADF recipe
- ionic liquid database

Selected features:

- COSMO-SAC and COSMO-RS models
- support for MOPAC
- import and export sigma profiles
- visualize sigma profiles and many properties
- improve predictions by adding pure compound data



COSMO-SAC: improved thermodynamic properties, Ind. Eng. Chem. Res., 53, 8265–8278 (2014).

Application areas

Academic research

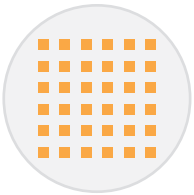
Industrial research

Teaching

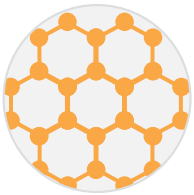
Whether you are an academic scrutinizing molecular properties, an industrial researcher designing the next generation material, or an enthusiastic computational chemistry teacher, we have the tools for you.

The ADF Modeling Suite is used by scientists in many different fields, in particular:

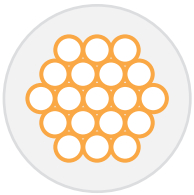
Inorganic chemistry



Organic electronics



Materials science



Nanoscience

Pharma

Oil & gas

Spectroscopy

Heavy elements

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Academic development

Excellent GUI

Expert support team

Parallel binaries

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