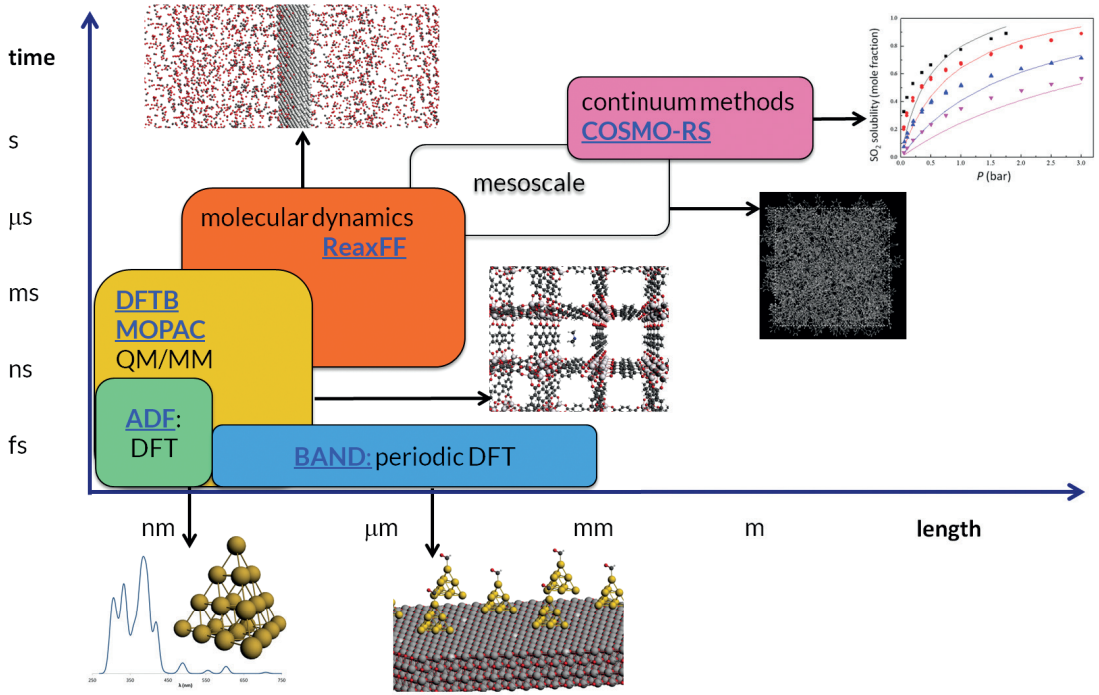
# ADF Modeling Suite

## Powerful Computational Chemistry

SCM
Software for
Chemistry &
Materials

# ADF Modeling Suite

**From molecules to materials, we make computational chemistry work for you!**
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.




**People behind the software**
ADF originated in the 1970s from the theoretical chemistry group at the VU University in Amsterdam, resulting in the foundation of SCM in 1995. Software for Chemistry & Materials has been steadily growing since then, and now has a team of about 20 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

**Expert support team**
Get excellent tech support from the software developers themselves. Also during your trial!

**Academic development**
Advance your research with the latest computational chemistry tools by our academic collaborations

**Excellent GUI**
Easily set up, run & analyze calculations with the powerful integrated GUI - on Mac, Windows & Linux

**Parallel binaries**
Accelerate your research with hassle-free installation of our out-of-the-box parallel binaries. Runs in the cloud, too

# Fully integrated graphical interface

The integrated graphical user interface (GUI) works with all our codes on Mac, Windows and Linux, which makes it easy to set up and visualize different job types.

## Build

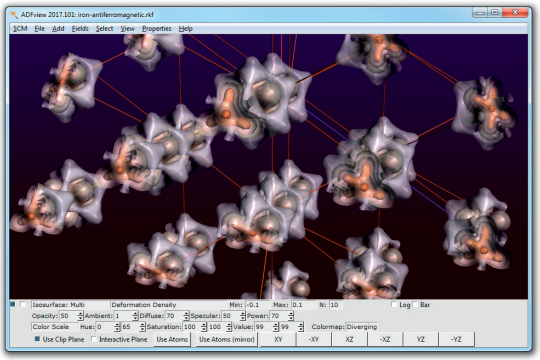
- import xyz, pdb, smiles, cif...
- large database of structures, complex mixtures with Packmol
- slice surfaces, create supercells
- easy toggling between clusters and periodic systems

## Run

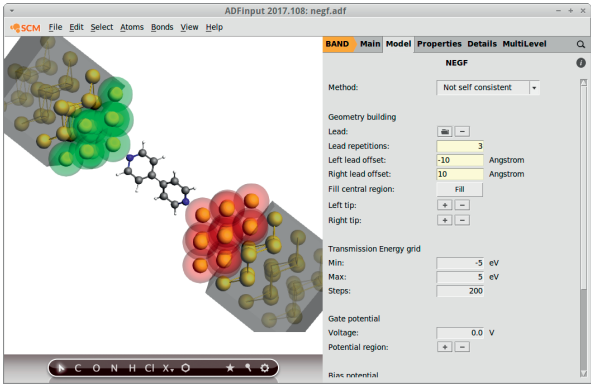
- cross-platform compatible, remote queues
- chained jobs, scripting, workflows

## Analyze

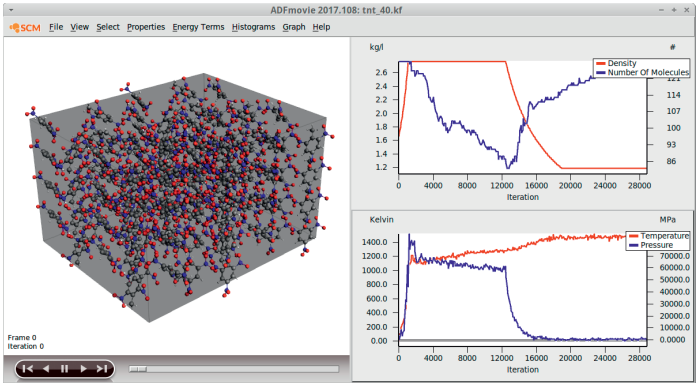
- quick visualization of MOs, densities, properties
- orbital level diagrams
- (partial) DOS, band structures, many spectra
- movies of vibrations, optimization, MD trajectories and properties



Easy to run Quantum Espresso and visualize with our GUI.




BAND: Electronic transport w. Non-Equilibrium Green's Functions.




ReaxFF: High rate impact sensitivity of TNT.

# ADF: molecular DFT

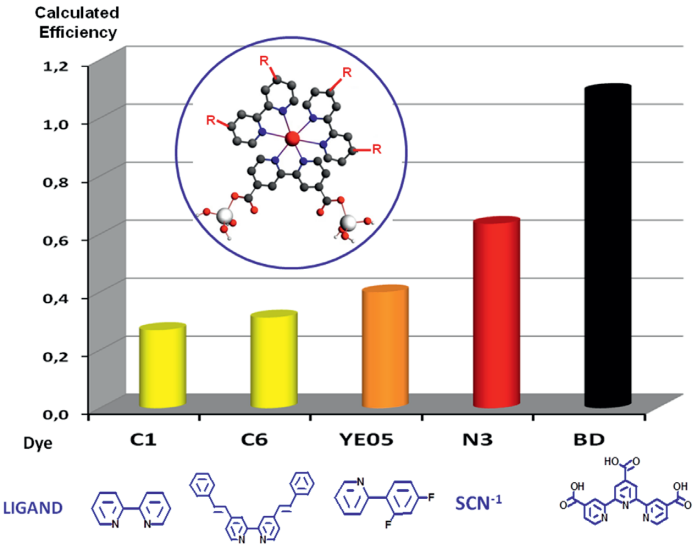
Our flagship program Amsterdam Density Functional (ADF) has a 40-year track record in handling the most diffcult problems in chemistry and materials science. ADF is accurate, fast, and robust software to study chemical reactivity, intricate bonding, and spectroscopic properties from simple to exotic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

## Strong points:

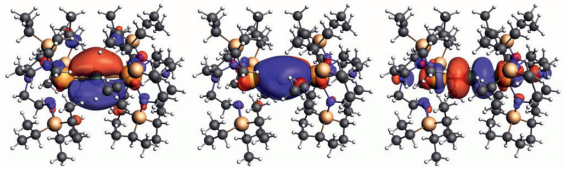
- accurate and efficient treatment of relativistic effects
- many spectroscopic properties from NMR to X-Ray
- insight in chemical bonding with detailed analysis
- advanced methods for including environment effects

## Selected features:

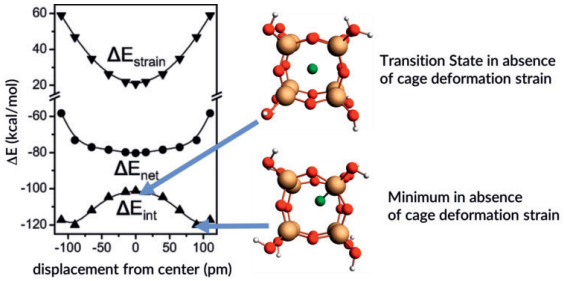
- phosphorescence lifetimes with spin-orbit coupling TDDFT
- charge mobilities with transfer integrals and NEGF
- modern functionals, including meta-GGAs, long-range corrected hybrids, dispersion corrections
- Slater orbitals describe core electronic properties better (NMR, EPR)
- easy scripting for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




Performance of ruthenium dyes in dye sensitized solar cells, J Mol. Model 22, 118 (2016).



Novel Thorium Arsenic Multiple Bonds, Nature Comm. 8, 14769 (2017).




8-Coordinate Fluoride in a Silicate Double-4-Ring, Proc. Nat. Acad. Sci. 114, online (2017).

# BAND: periodic DFT

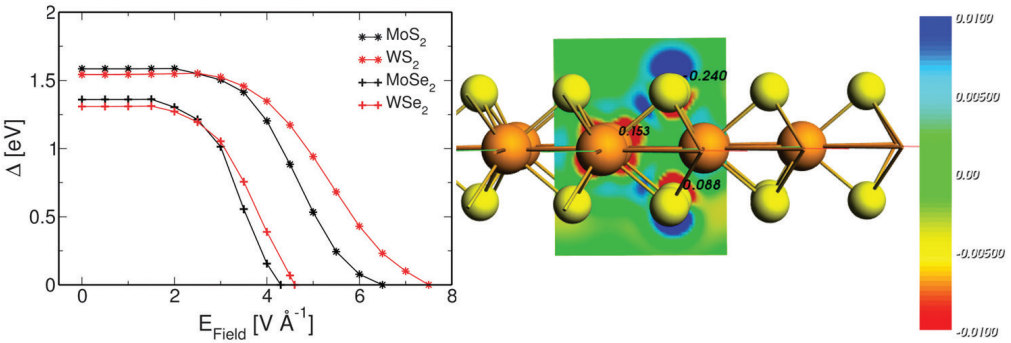
Our periodic DFT code BAND is a perfect companion to ADF, with the same basis sets and relativistic treatment. BAND is also strong in (core) electronic properties and analyzing orbitals and chemical bonds. It is particularly fast for low-dimensional and empty systems.

## Strong points:

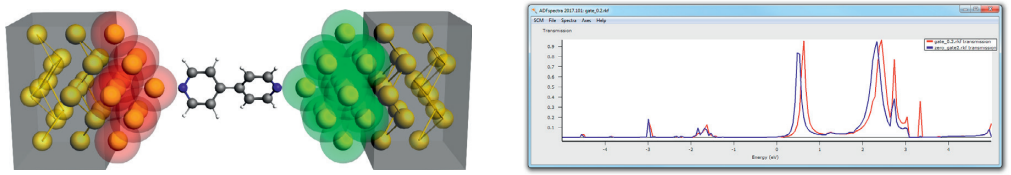
- easy to compare cluster and periodic with same basis sets
- spectroscopic properties, including core electrons (NMR, EPR, NEXAFS)
- real 1D and 2D: no artificial repetition in 3D
- all-electron basis sets for all elements: no pseudopotential approximation
- self-consistent spin-orbit coupling

## Selected features:

- continuum solvation: COSMO
- homogeneous electric fields / external magnetic fields
- analysis tools: orbitals, pEDA, (p)DOS, fat bands, QT-AIM, COOP, ELF
- modern functionals, including meta-GGAs, range-separated hybrids, dispersion corrections
- electronic transport with NEGF: gate and bias potentials, spin transport
- dielectric constant and function for bulk and surfaces




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



Non-equilibrium Green's function (NEGF): Au-(4,4'-bipyridine)-Au molecular junction

# DFTB, MOPAC: semi-empirical

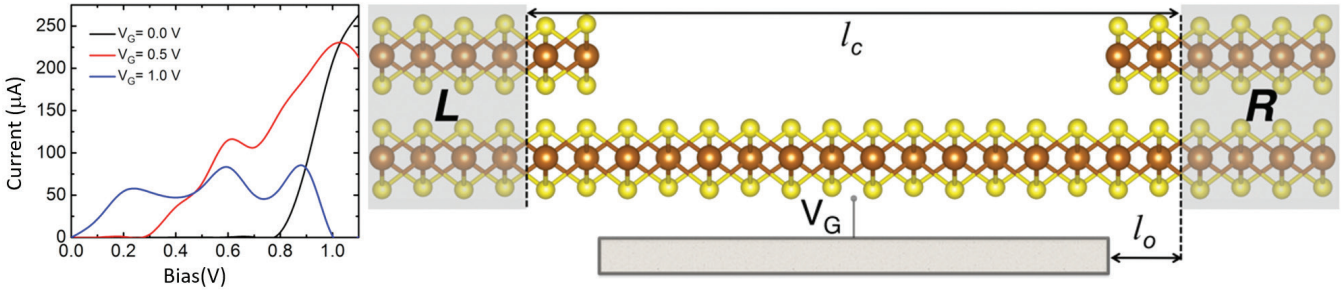
Our density-functional based tight binding (DFTB) and MOPAC are both fast codes which could bring the quantum precision you need to study large molecules or periodic systems. A good trade-off between speed and accuracy is achieved through a minimal basis and parameterization.

## Strong points:

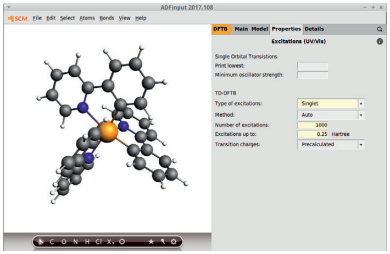
- quick pre-optimization, fast screening, and scriptable workflows
- molecules as well as proper 1D, 2D, and 3D periodicity
- most elements available for electronic DFTB and MOPAC
- easy incorporation in multi-layer models

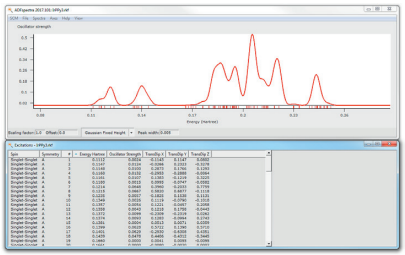
## Selected DFTB features:

- DFTB3 including dispersion corrections (D3-BJ)
- parameters: DFTB.org, Quasinano 2013 & 2015
- spectroscopy: IR, phonons, UV/VIS, Franck-Condon factors
- electronic transport with NEGF
- molecular dynamics
- orbital visualization




Logical junction from 2D PbS2 only, Adv. Mater. 2016, 10.1002/adma.201504274





UV/Vis spectrum of Ir(ppy)3 with SCC-TD-DFTB

# ReaxFF: reactive MD

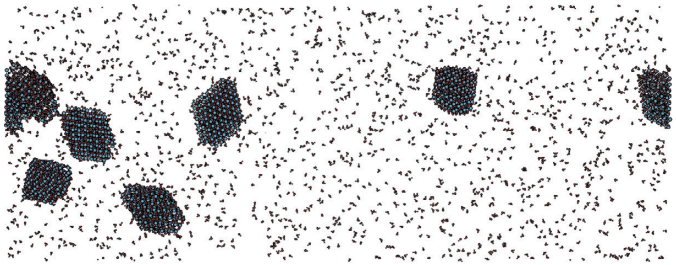
Study chemical reactions and molecular dynamics in large, complex systems with ReaxFF. We continue to improve usability and functionality in collaboration with Prof. van Duin and others. ReaxFF is applied in all areas of chemistry and materials science, most notably in combustion, batteries, glasses,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

## Strong points:

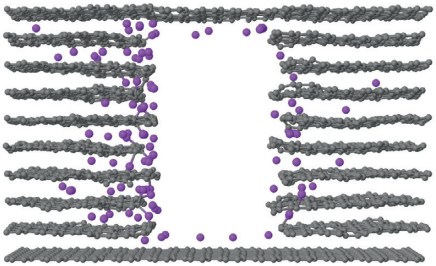
- easy building and set up of complex simulations
- analyze and visualize changing composition on the fly
- automated reaction path detection
- many force fields included, (re)parameterize with MCFF optimizer

## Selected ReaxFF features:

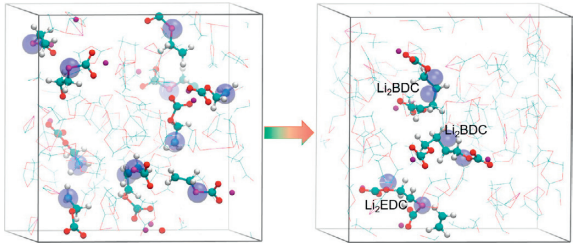
- NVT, NPT, NVE, non-reactive MD, optimization
- Nose-Hoover chains thermostat and barostats (isotropic, anisotropic and full cell fluctuation NPT)
- grand-canonical Monte Carlo: reactivity under equilibrium conditions
- accelerated reactive MD: (mass-scaled) force-biased Monte Carlo
- eReaxFF: pseudoclassical treatment of explicit electrons (batteries, redox reactions)



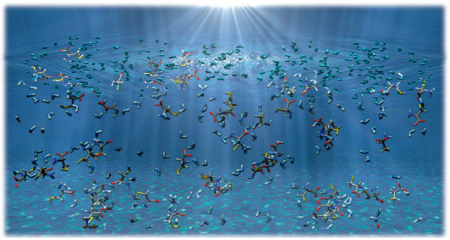
Oriented attachment of TiO2 nanocrystals, Nano Lett. 14, 1836-1842 (2014)



Sodium intrusion in graphitic cathodes
PCCP 18, 31431-31440 (2016)




Reductive Decomposition Reactions of Ethylene Carbonate
J. Phys. Chem. C, 120 (48), 27128–27134 (2016)



Surface-Altered Protonation of cysteine species in aqueous solution.
J. Phys. Chem. Lett. 6, 807–811 (2015)

# COSMO-RS: fluid thermodynamics

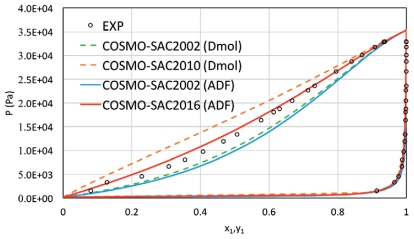
The COnductor-like Screening MOdel for Realistic Solvents calculates thermodynamic properties of fluids and solutions based on quantum mechanical data. COSMO-RS has predictive power for properties of all compounds, as opposed to group-based methods (e.g. UNIFAC) .

**Strong points:**

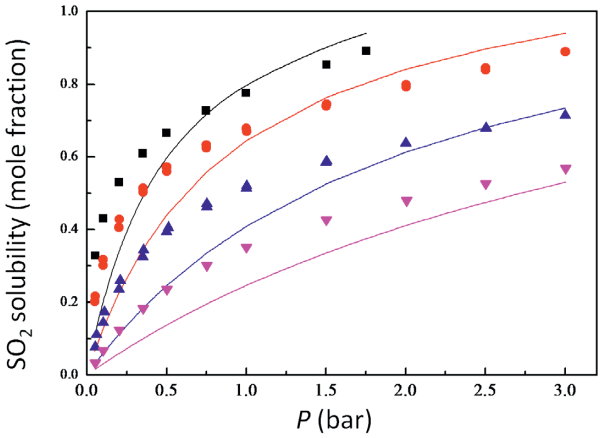
- predict many properties instantaneously (solubilities, logP, vapor-liquid equilibrium, ...)
- improved solvation energies and pKa values compared to COSMO
- quick property screening with scripting tools
- database of 1892 molecules, easy to expand with fixed ADF recipe
- ionic liquid database

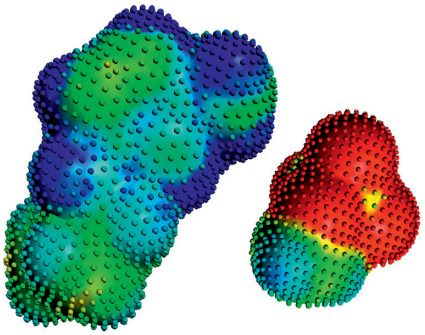
**Selected features:**

- 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 2016-ADF
from the group of S. T. Lin, based on:
Ind. Eng. Chem. Res. 55, 9312 (2016)




Gas Solubility in Ionic Liquids, Chem. Rev., 114, 1289−1326 (2014).

# Scripting

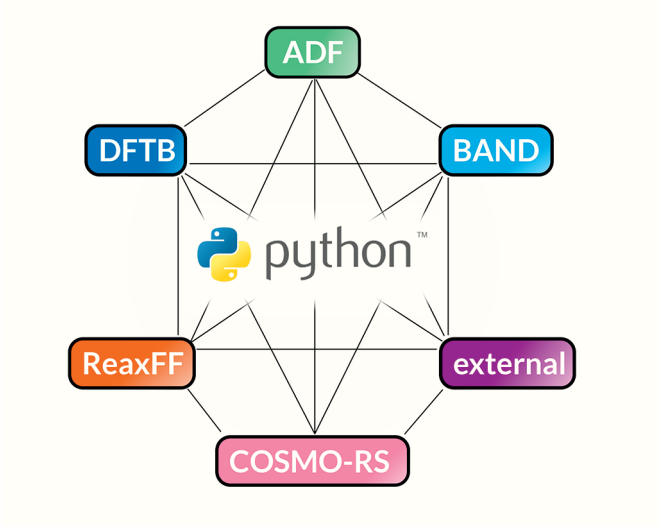
Whether you want to automatize simple recurring tasks, create your own screening workflows, or prototype a new method on top of ADF's computational engines, scripting is the right tool to get it done. Our open-source Python library PLAMS takes care of input preparation, (parallel) job execution, file management, and output processing for you. Combine PLAMS with RDKit for cheminformatics and machine learning applications. The FlexMD library offers scripting solutions in the field of multi-scale molecular dynamics and metadynamics simulations.
Find out more: https://www.scm.com/doc/Scripting/index.html

**Strong points:**

- no need to install anything: Python comes with every ADF program and is ready to use
- RDKit (Cheminformatics and Machine Learning), ASE
- FlexMD: Flexible multi-scale Molecular Dynamics simulation, e.g. adaptive QM/MM
- run interactively with IPython

**Selected PLAMS features:**

- parallel execution without the need to prepare special scripts
- integration with popular job schedulers (OGE, SLURM, TORQUE)
- manipulating molecular geometries
- full support for all ADFSuite programs and Dirac, Orca, CP2K, DFTB+,...
- open-source and easy extendable for other programs, job schedulers, file formats etc.




PLAMS

RDKit
Open-Source Cheminformatics and Machine Learning

IP[y]: IPython

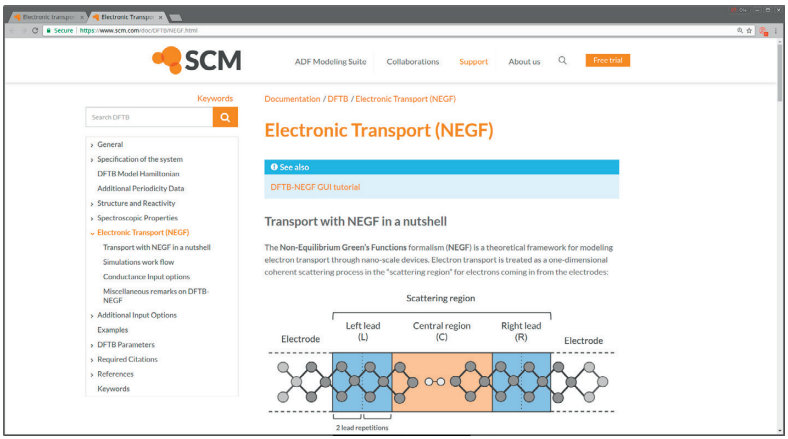
and many more...

# Application areas

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

- Inorganic chemistry
- Organic electronics
- Materials science
- Nanoscience
- Pharma
- Oil & gas
- Spectroscopy
- Heavy elements

# Getting started




DFTB-NEGF documentation

**Getting started is easy:**
Just visit our website www.scm.com to sign up for a free trial, browse through the tutorials or check where the next ADF workshop is given.

Explore the ADF Modeling Suite yourself:

www.scm.com/free-trial

## Powerful Computational Chemistry

Expert support team

Excellent GUI

Academic development

Parallel binaries

## Software for Chemistry & Materials

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