

# NEW IN ADF 2007

*The universal  
density functional  
package for chemists!*



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The Amsterdam Density Functional (ADF) brochure gives a general overview of ADF's capabilities. This leaflet focuses on improvements in the ADF2007 release of August 2007.

## The molecular ADF program

### Study of Potential Energy Surfaces

The delocalized coordinates geometry optimizer now works much better for weakly bound and floppy molecules, and for systems demanding tight convergence. This algorithm is also available for transition state (TS) searches. For TS searches, an analytic Hessian calculation for selected atoms that take an active part in the reaction provides a quick way to obtain a reliable start-up Hessian. The Nudged-Elastic-Band (NEB) implementation for TS search has also been improved, leading to fewer steps until convergence. For the validation of minima and saddle points, a frequency scan is now available also after an analytic frequency calculation.

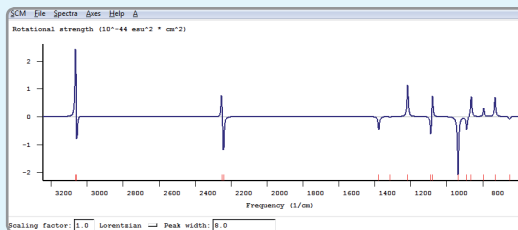
The introduction of energy gradients at the spin-orbit level means that energy surfaces for heavy element compounds can be studied more precisely.

The accurate MO6 class of xc energy functionals by Zhao and Truhlar have been implemented in post-SCF manner.

An alternative DIIS implementation during the SCF (NEWDIIS keyword) solves some cases with previously problematic SCF convergence.

### Spectroscopy

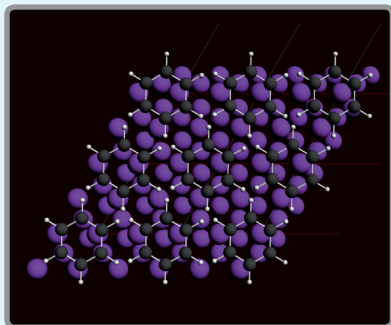
Vibrational Circular Dichroism (VCD) spectra and Raman spectra for selected normal modes can now both be calculated. The computational cost is only slightly higher than that of an analytic frequency calculation. Both types of spectra can be visualized with the ADFspectra GUI module.



*A visualization of the VCD spectrum of oxirane shown in the ADFspectra module.*

### Environment models

The Frozen Density Embedding (FDE) implementation has become more flexible and is ready for future additions for "subsystem DFT". The QUILD model (QUAntum regions Interconnected by Local Descriptions) is available. QUILD is an expert option allowing different computational models (e.g. different basis sets, different xc functionals, non-DFT methods) to be applied to different parts of the system.



## The periodic structure program BAND

A major step forward for BAND is the possibility to optimize geometries of polymers, (molecules on) surfaces, and solids.

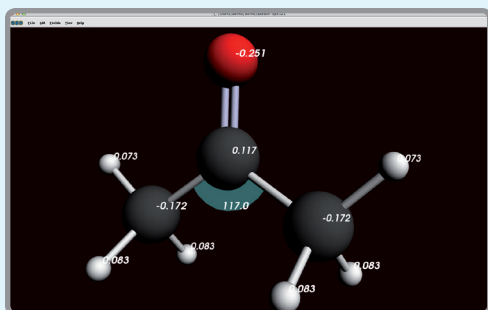
*With the BAND-GUI surface builder, it is now trivial to create a three layer Cu(111) slab, with a  $\sqrt{3} \times \sqrt{3}$  unit cell, or create a larger (2x2) surface with benzene adsorbed (see picture). BAND can now optimize structures for such systems.*

Because of several algorithmic improvements, BAND can now also deal with larger unit cells than before.

The time-dependent DFT implementation in BAND has been extended to describe metals and spin-orbit effects, and includes an implementation of the Vignale-Kohn kernel.

## The graphical user interfaces for ADF and BAND

A new module, ADFjobs, facilitates remote job submission and job management for ADF and BAND jobs. Other ADF-GUI improvements include the visualization of bond lengths and angles, and atomic charges, export of MPEG movies, energy graphs, import/export of cube files, as well as various usability and design improvements. The BAND-GUI now contains a crystal and surface builder.



*ADFview: atomic charges and the angle between three atoms*

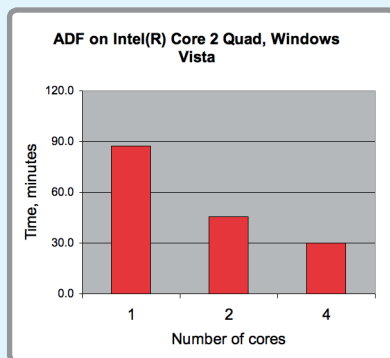
| Job              | Machine         | Status  |
|------------------|-----------------|---------|
| Crystals         | methione        |         |
| Crystals.methane | methione        |         |
| Crystals.najz    | methione        |         |
| exp              | methione        |         |
| propaan.popt     | methione        |         |
| methane          | localhost       |         |
| demon            | methione        |         |
| methaan.smi      | methione        |         |
| methaan.smi.141  |                 |         |
| Album            | methione        |         |
| propaan.demo     | TC 03 (0-15, 2) | 2       |
| propaan.demo     | methione        |         |
| hells            | opteron         |         |
| MOF_C120A        |                 |         |
| met              | MPX             |         |
| meton            | FXN 2-2         | 0:15:00 |
| Test Job         | sw              | 1-1     |

*ADFjobs: keeping track of your jobs on different machines*

## Parallel Windows version and HP-MPI

A parallel Windows version, which is trivial to install, leads to significant performance improvements on multi-core and multi-CPU Windows machines, and also supports Windows Vista.

*Our standard test calculation on a 105-atom Pt-compound runs in less than half an hour if all cores on a quad-core Windows Vista machine are used.*



The HP-MPI library is included in the ADF distribution for various platforms and simplifies ADF installation for many Linux cluster configurations and interconnects without recompilation.

## Free trial and further information

A free 30-day trial for ADF2007 is available on our website <http://www.scm.com>  
Feel free to contact us at [info@scm.com](mailto:info@scm.com) with any question.

## Literature references

- ADF - QUILD and optimizer improvements: Swart, M.; Bickelhaupt, F. M., J. Comput. Chem. 2007, accepted.
- ADF - Vibrational Circular Dichroism: V.P. Nicu, J. Neugebauer, S.K. Wolff, E.J. Baerends, Theor. Chem. Acc. DOI 10.1007/s00214-006-0234-x
- ADF - FDE rewrite: C.R. Jacob, J. Neugebauer, L. Visscher, 2007, submitted. Based on theory from T.A. Wesolowski, A. Warshel, J. Phys. Chem. 97, 8050 (1993)
- ADF - MO6 xc energy functionals: Y. Zhao, D.G. Truhlar, Theor. Chem. Acc., 2007, in press, <http://dx.doi.org/10.1007/s00214-007-0310-x>
- BAND - Energy gradients: E. S. Kadantsev, R. Klooster. P. L. de Boeij, and T. Ziegler, Mol. Phys. 2007, accepted.
- BAND - Time-Dependent DFT extensions: Ph.D. theses P. Romaniello and A. Berger available at <http://www.scm.com/Doc/theses.html>



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