References

ADF Program System
Release 2010

Scientific Computing & Modelling NV
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General References

When you publish results in the scientific literature that were obtained with programs of the ADF package, you are required to include references to the program package with the appropriate release number, and a few key publications.

In addition to these general references, references to special features are mandatory, in case you have used them. See the section Feature References ADF and Feature References BAND.

For ReaxFF calculations, include the relevant Force Field Reference in addition to the general ReaxFF references.

ADF

For calculations with the molecular ADF program, version 2010:


Optionally, you may add the following list of authors and contributors:


Note: if you have used a modified (by yourself, for instance) version of the code, you should mention in the citation that a modified version has been used.

BAND

For calculations with the periodic structures BAND program, version 2010:


Optionally, you may add the following list of authors and contributors:
P.H.T. Philipsen, G. te Velde, E.J. Baerends, J.A. Berger, P.L. de Boeij, J.A. Groeneveld, E.S.

Note: if you have used a modified (by yourself, for instance) version of the code, you should mention in the citation that a modified version has been used.

COSMO-RS

For calculations with the COSMO-RS program, version 2010:


   Optionally, you may add the following list of authors and contributors:
   J.N. Louwen, C.C. Pye, E. van Lenthe

ADF-GUI and BAND-GUI

The ADF-GUI and BAND-GUI have been developed within SCM (with O. Visser as primary developer). Main contributions outside SCM have come from:
P. Leyronnas, W.-J. van Zeist, and M. Luppi.

If you used the ADF-GUI (for example ADFview) you may optionally include the reference:


Likewise if you used the BAND-GUI you may optionally include the reference:


ReaxFF

The ReaxFF software that SCM makes available is based on the ReaxFF program developed by Adri van Duin.

For calculations with ReaxFF:


   Optionally, you may add the following list of authors and contributors:
   A.C.T. van Duin, W.A. Goddard

The ReaxFF GUI (ReaxFFinput and ADFmovie) has been developed within SCM (with O. Visser as primary developer).
The ReaxFF program has been optimized (much faster, running in parallel, and using shared memory) by SCM (with A.L. Yakovlev as primary developer).

If you use one of the included force fields you must also add the proper reference for it.

Many examples of ReaxFF applications can be found on Prof. van Duin's publication list.
Feature References ADF

When you have used special features, you should include one (or more, as the case may be) lead reference(s) to the implementation. Additional references to related publications are suggested.

Coordinates, basis sets, fragments

Basis Sets


Nuclear model

spherical Gaussian nuclear charge distribution model


Geometry optimizations, transition states, and reaction paths

Transition State search


IRC


Nudged Elastic Band


Quild

For calculations with the Quild program

**DFTB**

For calculations with the Density Functional Tight Binding (DFTB) program


   Optionally, you may add the author: D.A. McCormack

DFTB parameter files available in the ADF package


**Model Hamiltonians**

**Density Functional**

**OEP**


**Relativistic Effects**

**ZORA**

Lead references


Suggested related references


**Pauli**

**Lead references**


**Solvents and other environments**

**COSMO: Conductor like Screening Model**


**QM/MM: Quantum mechanical and Molecular Mechanics model**

**Lead**


**Suggested**


**For AddRemove model**


**FDE: Frozen Density Embedding**


**DRF: Discrete Solvent Reaction Field model**


**SCRF: Self-Consistent Reaction Field**


**3D-RISM: Three-Dimensional Reference Interaction Site Model**

**Lead**


**Suggested**


**MM Dispersion: Molecular Mechanics dispersion-corrected functionals**


**old implementation**


contact: J.M. Ducere, L. Cavallo, University of Salerno, Italy
Molecular properties with ADF

Frequencies, IR Intensities, Raman, VCD

Numerical Differentiation of Gradients


Analytical Second Derivatives


Mobile Block Hessian (MBH)

Lead


Suggested


(Resonance) Raman Scattering

Raman scattering


Resonance Raman: excited-state finite lifetime

Resonance Raman: excited-state gradient


VROA: (Resonance) vibrational Raman optical activity


Vibrational Circular Dichroism (VCD)


Franck-Condon factors


Time-Dependent DFT

For all Time-Dependent DFT features (Excitation Energies, (Hyper) Polarizabilities, Dispersion Coefficients, Raman Scattering, include:


Excitation Energies and Oscillator Strengths

Lead reference


Suggested (when ZORA relativistic results are used)


Open Shell ground state


Spin-flip transitions


Core excitations


Excitations including spin-orbit coupling


Perturbative approach to include spin-orbit coupling


Polarizabilities

Lead


Polarizabilities including spin-orbit coupling


Suggested


Hyperpolarizabilities

Lead


Suggested:
Dispersion Coefficients

Lead


Suggested


Circular Dichroism (CD)

Lead


Optical Rotation (OR), Optical Rotation Dispersion (ORD)

Lead


Magnetizability

Lead


Magnetic Circular Dichroism (MCD)


Verdet constant and Faraday term


NMR

NMR Chemical Shifts

Lead reference


NMR chemical shifts with hybrid functionals


NMR chemical shifts with NBO analysis


Suggested


**NMR spin-spin coupling**

**Lead**


**NMR spin-spin couplings with PBE0**


**NMR spin-spin couplings with NBO analysis**


**Suggested**


**Suggested book reference**


**ESR/EPR**

**G-tensor: Zeeman interaction**

Lead references (EPR/NMR program)


Lead reference (ADF)


**A-tensor: Nuclear magnetic dipole hyperfine interaction**

Lead reference


**Electric Field Gradient, NQCC**

Lead reference (in ESR called Q-tensor: Nuclear electric quadrupole hyperfine interaction)


EFG with NBO analysis


**Analysis**

**Bond Energy Analysis**

T. Ziegler and A. Rauk, *A theoretical study of the ethylene-metal bond in complexes between Cu\(^+\), Ag\(^+\), Au\(^+\), Pt\(^0\) or Pt\(^2+\) and ethylene, based on the Hartree-Fock-Slater transition-state method*. Inorganic Chemistry **18**, 1558 (1979)


ETS-NOCV

Feature References BAND

Lead

See key references above, for all work with BAND

Suggested


Geometry optimization

Lead


TDDFT

Lead


Main applications


P. Romaniello, P.L. de Boeij, F. Carbone, and D. van der Marel, *Optical properties of bcc transition metals in the range 0.40 eV*. Physical Review B 73, 075115 (2006)

Suggested book references


Relativistic TDDFT


Vignale Kohn

Lead


Applications


NMR

Lead


ESR

A-tensor: Nuclear magnetic dipole hyperfine interaction


G-tensor: Zeeman interaction

ReaxFF Force Field References

When you publish results in the scientific literature that were obtained with one of the included force fields for ReaxFF, including the proper reference for the force field used is mandatory.

AB (Ammonia Borane):


AuO:


CHO (Hydrocarbon oxidation):


Cu-water:


FeOCH:


HE (RDX/High Energy):


NaH:


NiCH:

VOCH:


ZnOH:


External programs and Libraries used by the ADF package

The next programs and/or libraries are used in the ADF package. On some platforms optimized libraries have been used and/or vendor specific MPI implementations.

Tcl/Tk

Description:
the scripting language used internally within the ADF package

Site:
http://www.tcl.tk/

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BSD-style open source license

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**Tcllib, including tklib (the Tcl standard library)**

Description:

standard library belonging to Tcl/Tk

Site:

http://www.tcl.tk/software/tcllib/

License:

BSD

On the TclTk wiki the following is mentioned about the license:

In response to popular demand, the Tcl core group is introducing tcllib, a Tcl standard library. This meta-package will contain many modules, each of which is itself a standalone Tcl package. The intention is to provide commonly used functions and libraries, bundled together under a single license (BSD), and with no binary dependencies.

The following text is included with both the tcllib and tklib distributions in license.terms:

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VTK

Description:
the visualization toolkit used by the GUI

Site:
http://www.vtk.org/

License:
BSD license

VTK is an open-source toolkit licensed under the BSD license.

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BLAS

Description:

Linear Algebra library

Site:

http://www.netlib.org/blas/

License:

unknown

The following information is from the BLAS FAQ on the mentioned site:

2) Are there legal restrictions on the use of BLAS reference implementation software?

The reference BLAS is a freely-available software package. It is available from netlib via anonymous ftp and the World Wide Web. Thus, it can be included in commercial software packages (and has been). We only ask that proper credit be given to the authors.

Like all software, it is copyrighted. It is not trademarked, but we do ask the following:

If you modify the source for these routines we ask that you change the name of the routine and comment the changes made to the original.

We will gladly answer any questions regarding the software. If a modification is done, however, it is the responsibility of the person who modified the routine to provide support.

LAPACK

Description:

Linear Algebra library

Site:

http://www.netlib.org/lapack/

License:

modified BSD

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**ScaLAPACK**

Description:

implementation of a subset of LAPACK routines for parallel computers

Site:

http://www.netlib.org/scalapack/

License:

modified BSD

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**Python 2.6**

Description:

scripting language

Site:

http://www.python.org/

License:

open source, GPL compatible

Click to read the license conditions printed by Python 2.6 by using the license() function.

**Numpy**

Description:

Library for scientific computing with Python

Site:
http://numpy.scipy.org/

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BSD License

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Open MPI

Description:

Open source MPI-2 implementation

Site:

http://www.open-mpi.org/

License:

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license.php:

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Platform MPI 7

Description:
High performance MPI implementation (formerly HP-MPI)

Site:
http://www.platform.com/Products/platform-mpi

License:
Commercial

OpenBabel

Description:
The Open Source Chemistry Toolbox
OpenBabel is used as an external command to convert input formats.

Site:
http://openbabel.org/

License:
GNU General Public License GPL2

Click to read the COPYING file as included with OpenBabel (the GPL2 license).

ASE

Description:
Atomistic Simulation Environment

ASE is used to perform MD simulations within pymd.

Site:

https://wiki.fysik.dtu.dk/ase/overview.html

Reference:

If you find ASE useful in your research please cite:

S. R. Bahn and K. W. Jacobsen
An object-oriented scripting interface to a legacy electronic structure code

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Packmol

Description:

Packing Optimization for Molecular Dynamics Simulations

Packmol (version of november 2009) is used to generate MD starting geometries. No changes
have been made to the source code, and the version of the source code that we have used is
included in $ADFHOME/Install/packmol.tar (november 2009).

Packmol is executed as an (external) stand-alone command via the GUI.

Site:

http://www.ime.unicamp.br/~martinez/packmol/

License:

GPL 3

Click to read the COPYING file as included with Packmol (the GPL3 license).
Following is the AUTHORS file as included with Packmol:
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Home-Page: http://www.ime.unicamp.br/~martinez/packmol

Symmol

Description:

Program to find symmetry of a molecule

Reference:


MEAD

Description:

Macroscopic Electrostatics with Atomic Detail

Site:

http://www.stjuderesearch.org/bashford-mead

Swish-e

Description:

Open source text-indexing tool

Starting with the 2011 release, Swish-e will be included and is used as an external program to search the documentation.

Site:

http://swish-e.org/

License:

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**FFTW**

Description:

Library to compute the discrete Fourier transform

Site:

http://www.fftw.org/

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