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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 2012:


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 2012:


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.
Ziegler

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.

**DFTB**

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

1. ADF DFTB 2012, SCM, Theoretical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands,
http://www.scm.com
   Optionally, you may add the following list of authors and contributors:
   Stefano Borini, Pier Philipsen, Alexei Yakovlev, Drew McCormack, Serguei Patchkovskii, Thomas Heine

If you use one of the included parameter sets you must also add the proper reference for it.

**MOPAC**

For calculations with MOPAC:

1. MOPAC2009, J. J. P. Stewart, Stewart Computational Chemistry; Colorado Springs, CO, USA
2. J. J. P. Stewart, Optimization of Parameters for Semiempirical Methods V: Modification of NDDO

**COSMO-RS**

For calculations with the COSMO-RS program, version 2012:

1. C.C. Pye, T. Ziegler, E. van Lenthe, J.N. Louwen, An implementation of the conductor-like screening
   model of solvation within the Amsterdam density functional package. Part II. COSMO for real solvents.
2. ADF2012 COSMO-RS, SCM, Theoretical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands,
   http://www.scm.com
   Optionally, you may add the following list of authors and contributors:
   J.N. Louwen, C.C. Pye, E. van Lenthe, E.S. McGarrity

**ReaxFF**

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

For calculations with ReaxFF:

1. A.C.T. van Duin, S. Dasgupta, F. Lorant, and W. A. Goddard, ReaxFF: A reactive force field for
2. K. Chenoweth, A.C.T. van Duin, and W.A. Goddard, ReaxFF reactive force field for molecular
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.

**GUI**

The integrated GUI has been developed by SCM (with O. Visser as primary developer), with some contributions from outside SCM (especially P. Leyronnas, W.-J. van Zeist, and M. Luppi).

If you used the GUI you may optionally include the reference:


**QUILD**

For calculations with the Quild program


**PyMD**

For calculations with PyMD:

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

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**


VSCRF (vertical excitation 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

F. Wang, T. Ziegler, E. van Lenthe, S.J.A. van Gisbergen and E.J. Baerends, The calculation of excitation energies based on the relativistic two-component zeroth-order regular approximation and

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


Paramagnetic NMR chemical shifts


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 reference (self-consistent spin-orbit coupling)


Lead reference (perturbative inclusion spin-orbit coupling)


Lead references (perturbative inclusion spin-orbit coupling with EPR/NMR program)


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

Lead reference


Lead reference (perturbative inclusion spin-orbit coupling)


**Electric Field Gradient, NQCC**

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


EFG with NBO analysis


**Transport properties: Non-self-consistent Green's function**

Chapter 2 and appendix C of

Analysis

Bond Energy Analysis

T. Ziegler and A. Rauk, *A theoretical study of the ethylene-metal bond in complexes between Cu⁺, Ag⁺, Au⁺, Pt⁰ or Pt²⁺ and ethylene, based on the Hartree-Fock-Slater transition-state method*. Inorganic Chemistry 18, 1558 (1979)

T. Ziegler and A. Rauk, *Carbon monoxide, carbon monosulfide, molecular nitrogen, phosphorus trifluoride, and methyl isocyanide as sigma donors and pi acceptors. A theoretical study by the Hartree-Fock-Slater transition-state method*. Inorganic Chemistry 18, 1755 (1979)


ETS-NOCV


QTAIM, Bader analysis

Grid-based algorithm

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):


HCONSB:


Cu-water:


FeOCH:


HE (RDX/High Energy):


NaH:


NiCH:


SiOH:


VOCH:


ZnOH:


DFTB Parameter References

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

mio-0-1 from DFTB.org

For systems containing O, N, C, H:

For systems also containing S:

mio-1-1 from DFTB.org

For systems containing O, N, C, H:

For systems also containing S:

For systems also containing P:

chalc-0-1 from DFTB.org

Include the DFTB.org/mio-0-1 references and add for As-S-H containing systems the chalc_0_1 reference:


matsci-0-3 from DFTB.org

The complete set:

For systems containing Al, O, and H:

For systems containing Al, Si, O, and H:

For systems containing Al, O, P, C, and H:
For systems containing Ti, O, P, C, and H:

For systems containing Ti, N, O, P, C, and H:

For systems containing Cu-Si, Cu-O, Cu-H, Na-H, Na-Si, Na-O:

miomod-hh-0-1 from DFTB.org
Modification of the DFTB.org/mio parameters for H-H potentials. Use appropriate mio references.

miomod-hn-0-1 from DFTB.org
Modification of the DFTB.org/mio parameters for N-H potentials. Use appropriate mio references and add for N-H:

pbc-0-3 from DFTB.org
For systems containing Si:

For systems containing Si and C:

For systems containing Si and O:

For systems containing F (and Si, O, N, C, H):

For systems containing F (and Si, O, N, C, H):

tiorg-0-1 from DFTB.org
In addition to the mio set, cite:

trans3d-0-1 from DFTB.org
In addition to the mio set, cite:
znorg-0-1 from DFTB.org

In addition to the mio set, cite:

Dresden


ThirdOrder


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/

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](http://www.python.org/) 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/

License:

BSD License

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IMPLIED WARRANTIES OF MERCHANTABILITY AND FITNESS FOR A PARTICULAR
PURPOSE ARE DISCLAIMED. IN NO EVENT SHALL THE COPYRIGHT OWNER OR
CONTRIBUTORS BE LIABLE FOR ANY DIRECT, INDIRECT, INCIDENTAL, SPECIAL,
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NEGLIGENCE OR OTHERWISE) ARISING IN ANY WAY OUT OF THE USE OF THIS
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Open MPI

Description:

Open source MPI-2 implementation

Site:

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

License:

New BSD License

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corresponding files.

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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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PLUMED

Description:

PLUMED is an open source plugin for free energy calculations in molecular systems.

Site:

http://www.plumed-code.org

Reference:

You may wish to cite the following reference if you have utilized PLUMED in your work:

Bonomi, D. Branduardi, G. Bussi, C. Camilloni, D. Provasi, P. Raiteri, D. Donadio, F. Marinelli, F.
Pietrucci, R.A. Broglia and M. Parrinello
PLUMED: a portable plugin for free-energy calculations with molecular dynamics, Comp. Phys.

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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:


Home-Page: http://www.ime.unicamp.br/~martinez/packmol

Symmol

Description:
Program to find symmetry of a molecule

Reference:

Symmol: T. Pilati and A. Forni, SYMMOL: *a program to find the maximum symmetry group in an atom cluster, given a prefixed tolerance*, Journal of Applied Crystallography 31, 503 (1998)

**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:

a modified version of GNU GPL2

Click to read the full license (taken from http://swish-e.org/license.html).

**FFTW**

Description:

Library to compute the discrete Fourier transform

Site:

http://www.fftw.org/

License:

commercial

**XCFun**

Description:
XCFun is a library of approximate exchange-correlation functionals

Site:

http://admol.org/xcfun

License:

A modified LGPL license that allows SCM to link statically with XCFun

The XCFun library is licensed under the LGPL license. This means that you may modify and distribute the library freely as long as you also release any changes made by you under the LGPL license. If you are just making modifications without distributing the modified library you are not obliged to release your changes. However, we do of course welcome all contributions as long as they are well tested and thought out

Reference:


**XQuartz**

Description:

A version of the X.Org X Window System that runs on OS X

The Mac OS X version (64 bit) uses XQuartz to run on Mountain Lion. The ADF2012.01.app application is a modified XQuartz.app, retaining the original copyright messages. The change is that after starting the Xserver the ADF-GUI application is automatically started.

Site:

http://xquartz.macosforge.org

License:

An XQuartz installation consists of many individual pieces of software which have various licenses. The X.Org software components' licenses are discussed on the X.Org Foundation Licenses page. The quartz-wm window manager included with the XQuartz distribution uses the Apple Public Source License Version 2.