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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 2013:


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 2013:


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, M. Franchini, J.A. Groeneveld,

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.

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:


COSMO-RS

For calculations with the COSMO-RS program, version 2013:


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

DFTB

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


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.

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, A.L. Yakovlev

The ReaxFF GUI (ReaxFFinput and ADFmovie) has been developed within SCM (with O. Visser as primary developer).

The ReaxFF program has been parallelized, optimized, and extended 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.

If you use special features, you must also add the proper references for them.

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

MOPAC

For calculations with MOPAC:

1. MOPAC2009, J. J. P. Stewart, Stewart Computational Chemistry; Colorado Springs, CO, USA

QUILD

For calculations with the Quild program


FlexMD

For calculations with FlexMD:


UFF

For calculations with the UFF4MOF parameters:

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

Range Separated Functionals


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**


**DIM/QM: Discrete Interaction Model/Quantum Mechanics**


**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


Perturbative approach to include spin-orbit coupling


**Excited state gradients**


**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

R.M. Dickson and T. Ziegler, *NMR Spin-Spin Coupling Constants from Density Functional Theory with Slater-Type Basis Functions*, Journal of Physical Chemistry 100, 5286 (1996)


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

Wide-band limit


**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**


**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

Feature and Force Field References ReaxFF

When you have used force fields or special features, you should include the reference(s) to the implementation.

Force-bias Monte Carlo (fbMC)


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:


CHONSSi-lg:

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 used DFT parameters 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 (same origin as Dresden parameters)

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:


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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, Cu-Na, 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):
C. Koehler, Th. Frauenheim, Molecular dynamics simulations of CFx (x = 2, 3) molecules at Si3N4 and SiO2 surfaces, Surf. Sci. 600, 453-460 (2003)

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

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

tiorg-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:

3ob-1-1 from DFTB.org

For systems containing O, N, C, H:

3ob-freq-1-1 from DFTB.org

Modified 3ob-parameters for vibrational frequencies:

3ob-hhmod-1-1 from DFTB.org

Modified H-H for 3ob (for H2):

3ob-nhmod-1-1 from DFTB.org

Modified N-H for 3ob (improves sp3-N proton affinities):

Dresden (same origin as matsci-0-3 parameters in DFTB.org)


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:

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.

Copyright (c) 1993-2008 Ken Martin, Will Schroeder, Bill Lorensen
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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/

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Python 2.6

Description:
scripting language

Site:
http://www.python.org/

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open source, GPL compatible

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Numpy

Description:
Library for scientific computing with Python

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

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Open MPI

Description:

Open source MPI-2 implementation

Site:

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

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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 FlexMD.

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:

=============================================

L. Martinez, R. Andrade, E. G. Birgin, J. M. Martinez,
Packmol: A package for building initial configurations for molecular dynamics simulations.

J. M. Martinez and L. Martinez,
Packing optimization for automated
generation of complex system’s initial configurations for molecular dynamics and docking.

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:

a modified version of GNU GPL2

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**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 ADF2013.01.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

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