Required citations

ADF Program System
Release 2014
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Feature and Force Field References

ReaxFF

Monte-Carlo force-field optimizer (MCFFOptimizer)

Boost Library

Verdet constant and Faraday term

NMR

NMR Chemical Shifts

NMR spin-spin coupling

ESR/EPR

G-tensor: Zeeman interaction

A-tensor: Nuclear magnetic dipole hyperfine interaction

Electric Field Gradient, NQCC

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

Analysis

Bond Energy Analysis

ETS-NOCV

QTAIM, Bader analysis

Accuracy and efficiency

Feature References BAND

Geometry optimization

TDDFT

Relativistic TDDFT

Vignale Kohn

NMR

ESR

Feature and Force Field References ReaxFF

Force-bias Monte Carlo (fbMC)

Grand Canonical Monte Carlo (GCMC)

Monte-Carlo force-field optimizer (MCFFOptimizer)

ReaxFF Force Field References

DFTB Parameter References

External programs and Libraries used by the ADF package

Tcl/Tk

Tcllib, including tklib (the Tcl standard library)

VTK

BLAS

LAPACK

ScalAPACK

Python 2.7

Numpy

SciPy

Open MPI

Platform MPI 7

OpenBabel

ASE

PLUMED

Packmol

Symmol

MEAD

Swish-e

FFTW

XCFun

XQuartz

RDKit

PRIMME library

Eigen library

PIL

Boost Library
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 2014:


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 2014:


   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.

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 2014:


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

If you use COSMO-SAC 2013-ADF you must also add


DFTB

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

   Optionally, you may add the following list of authors and contributors:
   Alexei Yakovlev, Pier Philipsen, Stefano Borini, Robert Rüger, Michiel de Reus, Mahdi Ghorbani Asl, Drew McCormack, Serguei Patchkovskii, Thomas Heine

For TD-DFTB, cite:
R. Rüger, E. van Lenthe, Y. Lu, J. Frenzel, T. Heine, and L. Visscher, Efficient Calculation of Electronic

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, H. van Schoot, 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. MOPAC2012, J.J.P. Stewart, Stewart Computational Chemistry; Colorado Springs, CO, USA


For parallel calculations, cite:


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

V.P. Osinga, S.J.A. van Gisbergen, J.G. Snijders and E.J. Baerends, *Density functional results for isotropic and anisotropic multipole polarizabilities and C\textsubscript{6}, C\textsubscript{7}, and C\textsubscript{8} Van der Waals dispersion coefficients for molecules*, Journal of Chemical Physics **106**, 5091 (1997)

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


Accuracy and efficiency

Numerical integration


Density fitting

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)**


**Grand Canonical Monte Carlo (GCMC)**


Thomas P. Senftle, Adri C.T. van Duin, Michael J. Janik, *Determining in situ phases of a nanoparticle catalyst via grand canonical Monte Carlo simulations with the ReaxFF potential*, Catalysis Communications volume 52, 5 July 2014, Pages 72–77

**Monte-Carlo force-field optimizer (MCFFOptimizer)**


**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.

Forcefields included in the ADF2014 release

Forcefields included in the development snapshots
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.

QUASINANO2013.1


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:

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):

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:

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.

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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 2.7

Description:

scripting language

Site:

http://www.python.org/

License:

open source, GPL compatible

Click to read the license conditions printed by Python 2.7 by using the license() function.

Numpy

Description:

Library for scientific computing with Python

Site:
http://www.numpy.org/

License:

BSD License

Numpy license
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SciPy

Description:

SciPy (pronounced “Sigh Pie”) is open-source software for mathematics, science, and engineering.

Site:

http://scipy.org/scipylib/

License:

BSD License

SciPy license
Copyright (c) 2001, 2002 Enthought, Inc.
All rights reserved.
Open MPI

Description:

Open source MPI-2 implementation

Site:

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

License:

New BSD License

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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
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:

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.stjude.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:

https://repo.ctcc.no/projects/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 ADF2014.01.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](http://xquartz.macosforge.org). The quartz-wm window manager included with the XQuartz distribution uses the Apple Public Source License Version 2.

RDKit

Description:

Open source toolkit for cheminformatics

The ADF-GUI uses RDKit to generate conformers, and to align and match conformers. In future versions more features from RDKit may be used.

Site:

http://www.rdkit.org/
License:

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PRIMME library

Description:

PRIMME: PReconditioned Iterative MultiMethod Eigensolver. SCM fixed some bugs in v1.1 of the PRIMME source, these changes have been communicated to the author and will be included in PRIMME v1.2. ADF2014 ships with a modified version of PRIMME v1.1, and is not backwards compatible. The modified sources can be downloaded below.

Site:

http://www.cs.wm.edu/~andreas/software/

Reference:

License:

LGPL 2.1

Click to read the license conditions included in the PRIMME source code.

Source code:

The source code of the PRIMME library v1.1 including the modifications by SCM can be downloaded here.

**Eigen library**

Description:

a lightweight C++ template library for linear algebra (used by RDKit)

Site:

http://eigen.tuxfamily.org/

License:

MPL v2.0

The following header is included with the Eigen library:

# This file is part of Eigen, a lightweight C++ template library
# for linear algebra.
#
# Copyright (C) 2012 Keir Mierle <mierle@gmail.com>
#
# This Source Code Form is subject to the terms of the Mozilla
# Public License v. 2.0. If a copy of the MPL was not distributed
# with this file, You can obtain one at http://mozilla.org/MPL/2.0/.
#
# Author: mierle@gmail.com (Keir Mierle)
#
# Make the long-awaited conversion to MPL.

**PIL**

Description:

Python Imaging Library (used by RDKit)

Site:

http://www.pythonware.com/products/pil/

License:
The Python Imaging Library is

Copyright (c) 1997-2009 by Secret Labs AB
Copyright (c) 1995-2009 by Fredrik Lundh

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Boost Library

Description:

Boost provides free peer-reviewed portable C++ source libraries (used by RDKit)

Site:

http://www.boost.org/

License:

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