



Scientific Computing & Modelling

Required citations

**ADF Program System
Release 2013**

Scientific Computing & Modelling NV
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Table of Contents

Required citations	1
Table of Contents	2
General References	4
ADF	4
BAND	4
GUI	5
COSMO-RS.....	5
DFTB.....	5
ReaxFF.....	5
MOPAC	6
QUILD	6
FlexMD.....	6
UFF.....	6
Feature References ADF	7
Coordinates, basis sets, fragments	7
Basis Sets.....	7
Nuclear model	7
Geometry optimizations, transition states, and reaction paths	7
Transition State search	7
IRC	7
Nudged Elastic Band.....	7
Model Hamiltonians	8
Density Functional	8
Range Separated Functionals	8
OEP	8
Relativistic Effects	8
ZORA.....	8
Pauli.....	8
Solvents and other environments	9
COSMO: Conductor like Screening Model	9
QM/MM: Quantum mechanical and Molecular Mechanics model	9
FDE: Frozen Density Embedding	9
DIM/QM: Discrete Interaction Model/Quantum Mechanics	9
SCRf: Self-Consistent Reaction Field	10
3D-RISM: Three-Dimensional Reference Interaction Site Model	10
MM Dispersion: Molecular Mechanics dispersion-corrected functionals	10
Molecular properties with ADF	11
Frequencies, IR Intensities, Raman, VCD.....	11
Numerical Differentiation of Gradients	11
Analytical Second Derivatives	11
Mobile Block Hessian (MBH).....	11
(Resonance) Raman Scattering	11
VROA: (Resonance) vibrational Raman optical activity	12
Vibrational Circular Dichroism (VCD)	12
Franck-Condon factors	12
Time-Dependent DFT.....	12
Excitation Energies and Oscillator Strengths	12
Excited state gradients	13
Polarizabilities.....	13
Hyperpolarizabilities	13
Dispersion Coefficients.....	14
Circular Dichroism (CD).....	14
Optical Rotation (OR), Optical Rotation Dispersion (ORD)	14
Magnetizability.....	14

Magnetic Circular Dichroism (MCD).....	15
Verdet constant and Faraday term.....	15
NMR.....	15
NMR Chemical Shifts.....	15
NMR spin-spin coupling.....	16
ESR/EPR.....	17
G-tensor: Zeeman interaction.....	17
A-tensor: Nuclear magnetic dipole hyperfine interaction.....	17
Electric Field Gradient, NQCC.....	17
Transport properties: Non-self-consistent Green's function.....	18
Analysis.....	18
Bond Energy Analysis.....	18
ETS-NOCV.....	18
QTAIM, Bader analysis.....	18
Feature References BAND.....	19
Geometry optimization.....	19
TDDFT.....	19
Relativistic TDDFT.....	20
Vignale Kohn.....	20
NMR.....	20
ESR.....	20
Feature and Force Field References ReaxFF.....	21
Force-bias Monte Carlo (fbMC).....	21
ReaxFF Force Field References.....	21
DFTB Parameter References.....	23
External programs and Libraries used by the ADF package.....	27
Tcl/Tk.....	27
Tcllib, including tklib (the Tcl standard library).....	28
VTK.....	29
BLAS.....	30
LAPACK.....	30
ScaLAPACK.....	31
Python 2.6.....	32
Numpy.....	32
Open MPI.....	33
Platform MPI 7.....	35
OpenBabel.....	35
ASE.....	35
PLUMED.....	36
Packmol.....	37
Symmol.....	37
MEAD.....	38
Swish-e.....	38
FFTW.....	38
XCFun.....	38
XQuartz.....	39

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:

1. G. te Velde, F.M. Bickelhaupt, S.J.A. van Gisbergen, C. Fonseca Guerra, E.J. Baerends, J.G. Snijders and T. Ziegler, *Chemistry with ADF*, [Journal of Computational Chemistry](#) **22**, 931 (2001)
2. C. Fonseca Guerra, J.G. Snijders, G. te Velde and E.J. Baerends, *Towards an order-N DFT method*, [Theoretical Chemistry Accounts](#) **99**, 391 (1998)
3. ADF2013, SCM, Theoretical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands, <http://www.scm.com>

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

E.J. Baerends, T. Ziegler, J. Autschbach, D. Bashford, A. Bérces, F.M. Bickelhaupt, C. Bo, P.M. Boerrigter, L. Cavallo, D.P. Chong, L. Deng, R.M. Dickson, D.E. Ellis, M. van Faassen, L. Fan, T.H. Fischer, C. Fonseca Guerra, M. Franchini, A. Ghysels, A. Giammona, S.J.A. van Gisbergen, A.W. Götz, J.A. Groeneveld, O.V. Gritsenko, M. Grüning, S. Gusarov, F.E. Harris, P. van den Hoek, C.R. Jacob, H. Jacobsen, L. Jensen, J.W. Kaminski, G. van Kessel, F. Kootstra, A. Kovalenko, M.V. Krykunov, E. van Lenthe, D.A. McCormack, A. Michalak, M. Mitoraj, S.M. Morton, J. Neugebauer, V.P. Nicu, L. Noodleman, V.P. Osinga, S. Patchkovskii, M. Pavanello, P.H.T. Philipsen, D. Post, C.C. Pye, W. Ravenek, J.I. Rodríguez, P. Ros, P.R.T. Schipper, G. Schreckenbach, J.S. Seldenthuis, M. Seth, J.G. Snijders, M. Solà, M. Swart, D. Swerhone, G. te Velde, P. Vernooijs, L. Versluis, L. Visscher, O. Visser, F. Wang, T.A. Wesolowski, E.M. van Wezenbeek, G. Wiesenekker, S.K. Wolff, T.K. Woo, A.L. Yakovlev

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:

1. G. te Velde and E.J. Baerends, *Precise density-functional method for periodic structures*, [Physical Review B](#) **44**, 7888 (1991)
2. G. Wiesenekker and E.J. Baerends, *Quadratic integration over the three-dimensional Brillouin zone*, [Journal of Physics: Condensed Matter](#) **3**, 6721 (1991)
3. BAND2013, SCM, Theoretical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands, <http://www.scm.com>

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,

E.S. Kadantsev, R. Klooster, F. Kootstra, P. Romaniello, D.G. Skachkov, J.G. Snijders, G. Wiesenekker, T. 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.

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:

GUI 2013, SCM, Amsterdam, The Netherlands, <http://www.scm.com>

COSMO-RS

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

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*, *Can. J. Chem.* **87**, 790 (2009)

2. ADF2013 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

DFTB

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

1. ADF DFTB 2013, 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 Philippsen, 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:

1. A.C.T. van Duin, S. Dasgupta, F. Lorant, and W. A. Goddard, *ReaxFF: A reactive force field for hydrocarbons*, *Journal of Physical Chemistry A* **105**, 9396-9409 (2001)

2. K. Chenoweth, A.C.T. van Duin, and W.A. Goddard, *ReaxFF reactive force field for molecular dynamics simulations of hydrocarbon oxidation*, *Journal of Physical Chemistry A* **112**, 1040-1053 (2008)

3. ReaxFF 2013, SCM, Theoretical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands, <http://www.scm.com>

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
2. J. J. P. Stewart, *Optimization of Parameters for Semiempirical Methods V: Modification of NDDO Approximations and Application to 70 Elements*, *J. Mol. Model.* **13**, 1173-1213 (2007)

QUILD

For calculations with the Quild program

M. Swart and F.M. Bickelhaupt, *QUILD: QUantum-regions interconnected by local descriptions*, *Journal of Computational Chemistry* **29**, 724 (2008)

FlexMD

For calculations with FlexMD:

1. FlexMD 2013, SCM, R. E. Bulo, C. R. Jacob, S. Borini, A python library for flexible multi-scale molecular dynamics simulations. <http://www.scm.com>

UFF

For calculations with the UFF4MOF parameters:

Matthew A. Addicoat, Nina Vankova, Ismot Farjana Akter, and Thomas Heine, *An extension of the Universal Force Field to Metal-Organic Frameworks*, *J. Chem. Theory Comput.* **10** (2), 880-891 (2013)

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

E. van Lenthe and E.J. Baerends, *Optimized Slater-type basis sets for the elements 1-118*, [Journal of Computational Chemistry](#) **24**, 1142 (2003)

Nuclear model

spherical Gaussian nuclear charge distribution model

J. Autschbach, *Magnitude of Finite-Nucleus-Size Effects in Relativistic Density Functional Computations of Indirect NMR Nuclear Spin-Spin Coupling Constants*, [ChemPhysChem](#) **10**, 2274 (2009)

Geometry optimizations, transition states, and reaction paths

Transition State search

L. Versluis and T. Ziegler, *The determination of Molecular Structure by Density Functional Theory*, [Journal of Chemical Physics](#) **88**, 322 (1988)

L. Fan and T. Ziegler, *Nonlocal density functional theory as a practical tool in calculations on transition states and activation energies*, [Journal of the American Chemical Society](#) **114**, 10890 (1992)

IRC

L. Deng, T. Ziegler and L. Fan, *A combined density functional and intrinsic reaction coordinate study on the ground state energy surface of H₂CO*, [Journal of Chemical Physics](#) **99**, 3823 (1993)

L. Deng and T. Ziegler, *The determination of Intrinsic Reaction Coordinates by density functional theory*, [International Journal of Quantum Chemistry](#) **52**, 731 (1994)

Nudged Elastic Band

G. Henkelman, B.P. Uberuaga and H. Jónsson, *A climbing image nudged elastic band method for finding saddle points and minimum energy paths*, [Journal of Chemical Physics](#) **113**, 9901 (2000)

Model Hamiltonians

Density Functional

Range Separated Functionals

M. Seth and T. Ziegler, *Range-Separated Exchange Functionals with Slater-Type Functions*, [Journal of Chemical Theory and Computation](#) **8**, 901 (2012)

OEP

M. Krykunov and T. Ziegler, *On the use of the exact exchange optimized effective potential method for static response properties*, [International Journal of Quantum Chemistry](#) **109**, 3246 (2009)

Relativistic Effects

ZORA

Lead references

E. van Lenthe, E.J. Baerends and J.G. Snijders, *Relativistic regular two-component Hamiltonians*, [Journal of Chemical Physics](#) **99**, 4597 (1993)

E. van Lenthe, E.J. Baerends and J.G. Snijders, *Relativistic total energy using regular approximations*, [Journal of Chemical Physics](#) **101**, 9783 (1994)

E. van Lenthe, A.E. Ehlers and E.J. Baerends, *Geometry optimization in the Zero Order Regular Approximation for relativistic effects*, [Journal of Chemical Physics](#) **110**, 8943 (1999)

Suggested related references

E. van Lenthe, J.G. Snijders and E.J. Baerends, *The zero-order regular approximation for relativistic effects: The effect of spin-orbit coupling in closed shell molecules*, [Journal of Chemical Physics](#) **105**, 6505 (1996)

E. van Lenthe, R. van Leeuwen, E.J. Baerends and J.G. Snijders, *Relativistic regular two-component Hamiltonians*, [International Journal of Quantum Chemistry](#) **57**, 281 (1996)

Pauli

Lead references

J.G. Snijders, E.J. Baerends and P. Ros, *A perturbation theory approach to relativistic calculations. II. Molecules*, [Molecular Physics](#) **38**, 1909 (1979)

P.M. Boerrigter, E.J. Baerends and J.G. Snijders, *A relativistic LCAO Hartree-Fock-Slater investigation of the electronic structure of the actinocenes $M(\text{COT})_2$, $M=\text{Th, Pa, U, Np}$ and Pu* , [Chemical Physics](#) **122**, 357 (1988)

T. Ziegler, V. Tschinke, E.J. Baerends, J.G. Snijders and W. Ravenek, *Calculation of bond energies in compounds of heavy elements by a quasi-relativistic approach*, [Journal of Physical Chemistry](#) **93**, 3050 (1989)

Solvents and other environments

COSMO: Conductor like Screening Model

C.C. Pye and T. Ziegler, *An implementation of the conductor-like screening model of solvation within the Amsterdam density functional package*, [Theoretical Chemistry Accounts](#) **101**, 396 (1999)

QM/MM: Quantum mechanical and Molecular Mechanics model

Lead

T. K. Woo, L. Cavallo and T. Ziegler, *Implementation of the IMOMM methodology for performing combined QM/MM molecular dynamics simulations and frequency calculations*, [Theoretical Chemistry Accounts](#) **100**, 307 (1998)

Suggested

T. K. Woo, S. Patchkovskii, and T. Ziegler, *Atomic Scale Modeling of Polymerization Catalysts*, [Computing in Science & Engineering](#), **2**, 28-37 (2000)

For AddRemove model

M. Swart, *AddRemove: A new link model for use in QM/MM studies*, [International Journal of Quantum Chemistry](#) **91**, 177 (2003)

FDE: Frozen Density Embedding

T.A. Wesolowski and A. Warshel, *Frozen Density Functional Approach for ab-initio Calculations of Solvated Molecules*, [Journal of Physical Chemistry](#) **97**, 8050 (1993)

J. Neugebauer, C.R. Jacob, T.A. Wesolowski and E.J. Baerends, *An Explicit Quantum Chemical Method for Modeling Large Solvation Shells Applied to Aminocoumarin C151* [Journal of Physical Chemistry A](#) **109**, 7805 (2005)

C.R. Jacob, J. Neugebauer and L. Visscher, *A flexible implementation of frozen-density embedding for use in multilevel simulations*, [Journal of Computational Chemistry](#) **29**, 1011 (2008)

DIM/QM: Discrete Interaction Model/Quantum Mechanics

J.L. Payton, S.M. Morton, Justin E. Moore, and Lasse Jensen, *A discrete interaction model/quantum mechanical method for simulating surface-enhanced Raman spectroscopy*, [Journal of Chemical Physics](#) **136**, 214103 (2012)

DRF: Discrete Solvent Reaction Field model

L. Jensen, P.T. van Duijnen and J.G. Snijders, *A discrete solvent reaction field model within density functional theory* [Journal of Chemical Physics](#) **118**, 514 (2003)

SCRF: Self-Consistent Reaction Field

J.L. Chen, L. Noodleman, D.A. Case and D. Bashford, *Incorporating solvation effects into density functional electronic structure calculations*, [Journal of Physical Chemistry](#) **98**, 11059 (1994)

VSCRF (vertical excitation self-consistent reaction field)

T. Liu, W.-G Han, F. Himo, G.M. Ullmann, D. Bashford, A. Toutchkine, K.M. Hahn, and L. Noodleman, *Density Functional Vertical Self-Consistent Reaction Field Theory for Solvatochromism Studies of Solvent-Sensitive Dyes*, [Journal of Physical Chemistry A](#) **108**, 3545 (2004)

W.-G. Han, T. Liu, F. Himo, A. Toutchkine, D. Bashford, K.M. Hahn, L. Noodleman, *A Theoretical Study of the UV/Visible Absorption and Emission Solvatochromic Properties of Solvent-Sensitive Dyes*, [ChemPhysChem](#) **4**, 1084 (2003)

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

Lead

S. Gusarov, T. Ziegler, and A. Kovalenko, *Self-Consistent Combination of the Three-Dimensional RISM Theory of Molecular Solvation with Analytical Gradients and the Amsterdam Density Functional Package*, [Journal of Physical Chemistry A](#) **110**, 6083 (2006)

Suggested

A. Kovalenko and F. Hirata, *Self-consistent description of a metal-water interface by the Kohn-Sham density functional theory and the three-dimensional reference interaction site model*, [Journal of Chemical Physics](#) **110**, 10095 (1999)

A. Kovalenko, *Three-dimensional RISM theory for molecular liquids and solid-liquid interfaces*, In *Molecular Theory of Solvation*; Hirata, Fumio, Ed.; Understanding Chemical Reactivity (series); Mezey, Paul G., Series Ed.; Kluwer Academic Publishers: Dordrecht, The Netherlands, 2003; Vol. 24, pp 169-275.

MM Dispersion: Molecular Mechanics dispersion-corrected functionals

S. Grimme, *Semiempirical GGA-Type Density Functional Constructed with a Long-Range Dispersion Correction*, [Journal of Computational Chemistry](#) **27**, 1787 (2006)

old implementation

S. Grimme, *Accurate description of van der Waals complexes by density functional theory including empirical corrections*, [Journal of Computational Chemistry](#) **25**, 1463 (2004)

J.-M. Duc  re and L. Cavallo, *Parametrization of an Empirical Correction Term to Density Functional Theory for an Accurate Description of pi-Stacking Interactions in Nucleic Acids*, [Journal of Physical Chemistry B](#) **111**, 13124 (2007)

contact: J.M. Ducere, L. Cavallo, University of Salerno, Italy

Molecular properties with ADF

Frequencies, IR Intensities, Raman, VCD

Numerical Differentiation of Gradients

L. Fan and T. Ziegler, *Application of density functional theory to infrared absorption intensity calculations on main group molecules*, [Journal of Chemical Physics](#) **96**, 9005 (1992)

L. Fan and T. Ziegler, *Application of density functional theory to infrared absorption intensity calculations on transition-metal carbonyls*, [Journal of Physical Chemistry](#) **96**, 6937 (1992)

Analytical Second Derivatives

A. Bérces, R. M. Dickson, L. Fan, H. Jacobsen, D. Swerhone and T. Ziegler, *An implementation of the coupled perturbed Kohn-Sham equations: perturbation due to nuclear displacements*, [Computer Physics Communications](#) **100**, 247 (1997)

H. Jacobsen, A. Bérces, D. Swerhone and T. Ziegler, *Analytic second derivatives of molecular energies: a density functional implementation*, [Computer Physics Communications](#) **100**, 263 (1997)

S. K. Wolff, *Analytical second derivatives in the Amsterdam density functional package*, [International Journal of Quantum Chemistry](#) **104**, 645 (2005)

Mobile Block Hessian (MBH)

Lead

A. Ghysels, D. Van Neck, V. Van Speybroeck, T. Verstraelen and M. Waroquier, *Vibrational Modes in partially optimized molecular systems* [Journal of Chemical Physics](#) **126**, 224102 (2007)

Suggested

A. Ghysels, D. Van Neck and M. Waroquier, *Cartesian formulation of the Mobile Block Hessian Approach to vibrational analysis in partially optimized systems* [Journal of Chemical Physics](#) **127**, 164108 (2007)

(Resonance) Raman Scattering

Raman scattering

S.J.A. van Gisbergen, J.G. Snijders and E.J. Baerends, *Application of time-dependent density functional response theory to Raman scattering*, [Chemical Physics Letters](#) **259**, 599 (1996)

S.J.A. van Gisbergen, J.G. Snijders and E.J. Baerends, *Implementation of time-dependent density functional response equations*, [Computer Physics Communications](#) **118**, 119 (1999)

Resonance Raman: excited-state finite lifetime

L. Jensen, L. Zhao, J. Autschbach and G.C. Schatz, *Theory and method for calculating resonance Raman scattering from resonance polarizability derivatives*, [Journal of Chemical Physics](#) **123**, 174110 (2005)

Resonance Raman: excited-state gradient

J. Neugebauer, E.J. Baerends, E. Efremov, F. Ariese and C. Gooijer, *Combined Theoretical and Experimental Deep-UV Resonance Raman Studies of Substituted Pyrenes*, [Journal of Physical Chemistry A](#) **109**, 2100 (2005)

VROA: (Resonance) vibrational Raman optical activity

L. Jensen, J. Autschbach, M. Krykunov, and G.C. Schatz, *Resonance vibrational Raman optical activity: A time-dependent density functional theory approach*, [Journal of Chemical Physics](#) **127**, 134101 (2007)

Vibrational Circular Dichroism (VCD)

V.P. Nicu J. Neugebauer S.K. Wolff and E.J. Baerends, *A vibrational circular dichroism implementation within a Slater-type-orbital based density functional framework and its application to hexa- and heptahelicenes*, [Theoretical Chemical Accounts](#) **119**, 245 (2008)

Franck-Condon factors

J.S. Seldenthuis, H.S.J. van der Zant, M.A. Ratner and J.M. Thijssen, *Vibrational Excitations in Weakly Coupled Single-Molecule Junctions: A Computational Analysis*, [ACS Nano](#) **2**, 1445 (2008)

Time-Dependent DFT

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

S.J.A. van Gisbergen, J.G. Snijders and E.J. Baerends, *Implementation of time-dependent density functional response equations*, [Computer Physics Communications](#) **118**, 119 (1999)

Excitation Energies and Oscillator Strengths

Lead reference

S.J.A. van Gisbergen, J.G. Snijders and E.J. Baerends, *Implementation of time-dependent density functional response equations*, [Computer Physics Communications](#) **118**, 119 (1999)

Suggested (when ZORA relativistic results are used)

A. Rosa, E.J. Baerends, S.J.A. van Gisbergen, E. van Lenthe, J.A. Groeneveld and J. G. Snijders, *Article Electronic Spectra of $M(\text{CO})_6$ ($M = \text{Cr}, \text{Mo}, \text{W}$) Revisited by a Relativistic TDDFT Approach*, [Journal of the American Chemical Society](#) **121**, 10356 (1999)

Open Shell ground state

F. Wang and T. Ziegler, [Mol. Phys.](#) **102**, 2585 (2004)

Spin-flip transitions

F. Wang and T. Ziegler, *Time-dependent density functional theory based on a noncollinear formulation of the exchange-correlation potential*, [Journal of Chemical Physics](#) **121**, 12191 (2004)

F. Wang and T. Ziegler, *The performance of time-dependent density functional theory based on a noncollinear exchange-correlation potential in the calculations of excitation energies*, [Journal of Chemical Physics](#) **122**, 74109 (2005)

Core excitations

M. Stener, G. Fronzoni and M. de Simone, *Time dependent density functional theory of core electrons excitations*, [Chemical Physics Letters](#) **373**, 115 (2003)

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 time-dependent density-functional with full use of symmetry*, [Journal of Chemical Physics](#) **122**, 204103 (2005)

Perturbative approach to include spin-orbit coupling

F. Wang and T. Ziegler, *A simplified relativistic time-dependent density-functional theory formalism for the calculations of excitation energies including spin-orbit coupling effect*, [Journal of Chemical Physics](#) **123**, 154102 (2005)

Excited state gradients

M. Seth, G. Mazur, and T. Ziegler, *Time-dependent density functional theory gradients in the Amsterdam density functional package: geometry optimizations of spin-flip excitations*, [Theoretical Chemistry Accounts](#) **129**, 331 (2011)

Polarizabilities

Lead

S.J.A. van Gisbergen, J.G. Snijders and E.J. Baerends, *A Density Functional Theory study of frequency-dependent polarizabilities and van der Waals dispersion coefficients for polyatomic molecules*, [Journal of Chemical Physics](#) **103**, 9347 (1995)

Polarizabilities including spin-orbit coupling

A. Devarajan, A. Gaenko, and J. Autschbach, *Two-component relativistic density functional method for computing nonsingular complex linear response of molecules based on the zeroth order regular approximation*, [Journal of Chemical Physics](#) **130**, 194102 (2009)

Suggested

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_6 , C_7 , and C_8 Van der Waals dispersion coefficients for molecules*, [Journal of Chemical Physics](#) **106**, 5091 (1997)

Hyperpolarizabilities

Lead

S.J.A. van Gisbergen, J.G. Snijders and E.J. Baerends, *Calculating frequency-dependent hyperpolarizabilities using time-dependent density functional theory*, [Journal of Chemical Physics](#) **109**, 10644 (1998)

Suggested:

S.J.A. van Gisbergen, J.G. Snijders, and E.J. Baerends, *Time-dependent Density Functional Results for the Dynamic Hyperpolarizability of C₆₀*, [Physical Review Letters](#) **78**, 3097 (1997)

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 C₆, C₇, and C₈ Van der Waals dispersion coefficients for molecules*, [Journal of Chemical Physics](#) **106**, 5091 (1997)

Suggested

S.J.A. van Gisbergen, J.G. Snijders and E.J. Baerends, *A Density Functional Theory study of frequency-dependent polarizabilities and van der Waals dispersion coefficients for polyatomic molecules*, [Journal of Chemical Physics](#) **103**, 9347 (1995)

Circular Dichroism (CD)

Lead

J. Autschbach and T. Ziegler, *Calculating molecular electric and magnetic properties from time-dependent density functional response theory*, [Journal of Chemical Physics](#) **116**, 891 (2002)

J. Autschbach, T. Ziegler, S.J.A. van Gisbergen and E.J. Baerends, *Chiroptical properties from time-dependent density functional theory. I. Circular dichroism spectra of organic molecules*, [Journal of Chemical Physics](#) **116**, 6930 (2002)

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

Lead

J. Autschbach and T. Ziegler, *Calculating molecular electric and magnetic properties from time-dependent density functional response theory*, [Journal of Chemical Physics](#) **116**, 891 (2002)

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

Modified 3ob-parameters for vibrational frequencies:

M. Gaus, A. Goez, M. Elstner *Parametrization and Benchmark of DFTB3 for Organic Molecules* *J. Chem. Theory Comput* **9**, 338-354 (2013)

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

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

M. Gaus, A. Goez, M. Elstner *Parametrization and Benchmark of DFTB3 for Organic Molecules* *J. Chem. Theory Comput* **9**, 338-354 (2013)

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

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

M. Gaus, A. Goez, M. Elstner *Parametrization and Benchmark of DFTB3 for Organic Molecules* *J. Chem. Theory Comput* **9**, 338-354 (2013)

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

J. Frenzel, A. F. Oliveira, N. Jardillier, T. Heine, G. Seifert, *Semi-relativistic, self-consistent charge Slater-Koster tables for density-functional based tight-binding (DFTB) for materials science simulations*, TU-Dresden **2004-2009**

J. Frenzel, A. F. Oliveira, H. A. Duarte, T. Heine, G. Seifert, *Structural and electronic properties of bulk gibbsite and gibbsite surfaces*, *Z. Anorg. Allg. Chem.* **631**, 1267-1271 (2005)

L. Guimaraes, A. N. Enyashin, J. Frenzel, T. Heine, H. A. Duarte, G. Seifert, *Imogolite Nanotubes: Stability, electronic and mechanical properties*, *Nano* **1**, 362-368 (2007)

R. Luschtinetz, A. F. Oliveira, J. Frenzel, J. Joswig, G. Seifert, H. A. Duarte, *Adsorption of phosphonic and ethylphosphonic acid on aluminum oxide surfaces*, *Surf. Sci.* **602**, 1347-1359 (2008)

R. Luschtinetz, J. Frenzel, T. Milek, G. Seifert *Adsorption of phosphonic acid at the TiO₂ anatase (101) and rutile (110) surface*, *J. Phys. Chem. C* **113**, 5730-5740 (2009)

ThirdOrder

M. Elstner, D. Porezag, G. Jungnickel, J. Elstner, M. Haugk, Th. Frauenheim, S. Suhai, G. Seifert, *Self-consistent-charge density-functional tight-binding method for simulations of complex materials properties*, *Phys. Rev. B* **58**, 7260-7268 (1998)

T. A. Niehaus, M. Elstner, Th. Frauenheim, S. Suhai, *Application of an approximate density-functional method to sulfur containing compounds*, *J. Mol. Struct. (THEOCHEM)* **541**, 185-194 (2001)

M. Gaus, Q. Cui, M. Elstner, *DFTB3: Extension of the Self-Consistent-Charge Density-Functional Tight-Binding Method (SCC-DFTB)*, [J. Chem. Theory Comput.](#) **7**, 931-948 (2011)

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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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.

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VTK

Description:

the visualization toolkit used by the GUI

Site:

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BLAS

Description:

Linear Algebra library

Site:

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

License:

unknown

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LAPACK

Description:

Linear Algebra library

Site:

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

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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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Description:

scripting language

Site:

<http://www.python.org/>

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Library for scientific computing with Python

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Platform MPI 7

Description:

High performance MPI implementation (formerly HP-MPI)

Site:

<http://www.platform.com/Products/platform-mpi>

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OpenBabel

Description:

The Open Source Chemistry Toolbox

OpenBabel is used as an external command to convert input formats.

Site:

<http://openbabel.org/>

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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

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Comput. Sci. Eng., Vol. **4**, 56-66, 2002

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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/>

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Packmol: A package for building initial configurations for molecular dynamics simulations.
[Journal of Computational Chemistry](#), **30** (13): 2157-2164 (2009).

J. M. Martinez and L. Martinez,
Packing optimization for automated generation of complex system's initial configurations for molecular dynamics and docking.
[Journal of Computational Chemistry](#), **24** (7): 819-825 (2003).

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.

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Library to compute the discrete Fourier transform

Site:

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Reference:

Ulf Ekström, Lucas Visscher, Radovan Bast, Andreas J. Thorvaldsen and Kenneth Ruud, *Arbitrary-Order Density Functional Response Theory from Automatic Differentiation*, *Journal of Chemical Theory and Computation* **6**, 1971 (2010), DOI: [10.1021/ct100117s](https://doi.org/10.1021/ct100117s)

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.

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