



Scientific Computing & Modelling

Required citations

**ADF Program System
Release 2014**

Scientific Computing & Modelling NV
Vrije Universiteit, Theoretical Chemistry
De Boelelaan 1083; 1081 HV Amsterdam; The Netherlands
WWW: www.scm.com
E-mail: support@scm.com

Copyright © 1993-2014: SCM / Vrije Universiteit, Theoretical Chemistry, Amsterdam, The Netherlands
All rights reserved

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.....	6
MOPAC	6
QUILD	6
FlexMD.....	7
UFF.....	7
Feature References ADF	8
Coordinates, basis sets, fragments	8
Basis Sets.....	8
Nuclear model	8
Geometry optimizations, transition states, and reaction paths	8
Transition State search	8
IRC	8
Nudged Elastic Band.....	8
Model Hamiltonians	9
Density Functional	9
Range Separated Functionals	9
OEP	9
Relativistic Effects	9
ZORA.....	9
Pauli.....	9
Solvents and other environments	10
COSMO: Conductor like Screening Model	10
QM/MM: Quantum mechanical and Molecular Mechanics model	10
FDE: Frozen Density Embedding	10
DIM/QM: Discrete Interaction Model/Quantum Mechanics	10
SCRf: Self-Consistent Reaction Field	11
3D-RISM: Three-Dimensional Reference Interaction Site Model	11
MM Dispersion: Molecular Mechanics dispersion-corrected functionals	11
Molecular properties with ADF	12
Frequencies, IR Intensities, Raman, VCD.....	12
Numerical Differentiation of Gradients	12
Analytical Second Derivatives	12
Mobile Block Hessian (MBH).....	12
(Resonance) Raman Scattering	12
VROA: (Resonance) vibrational Raman optical activity	13
Vibrational Circular Dichroism (VCD)	13
Franck-Condon factors	13
Time-Dependent DFT	13
Excitation Energies and Oscillator Strengths	13
Excited state gradients	14
Polarizabilities.....	14
Hyperpolarizabilities	14
Dispersion Coefficients.....	15
Circular Dichroism (CD).....	15
Optical Rotation (OR), Optical Rotation Dispersion (ORD)	15
Magnetizability.....	15

Magnetic Circular Dichroism (MCD).....	16
Verdet constant and Faraday term.....	16
NMR.....	16
NMR Chemical Shifts.....	16
NMR spin-spin coupling.....	17
ESR/EPR.....	18
G-tensor: Zeeman interaction.....	18
A-tensor: Nuclear magnetic dipole hyperfine interaction.....	18
Electric Field Gradient, NQCC.....	18
Transport properties: Non-self-consistent Green's function.....	19
Analysis.....	19
Bond Energy Analysis.....	19
ETS-NOCV.....	19
QTAIM, Bader analysis.....	19
Accuracy and efficiency.....	20
Feature References BAND.....	21
Geometry optimization.....	21
TDDFT.....	21
Relativistic TDDFT.....	22
Vignale Kohn.....	22
NMR.....	22
ESR.....	22
Feature and Force Field References ReaxFF.....	23
Force-bias Monte Carlo (fbMC).....	23
Grand Canonical Monte Carlo (GCMC).....	23
Monte-Carlo force-field optimizer (MCFFOptimizer).....	23
ReaxFF Force Field References.....	23
DFTB Parameter References.....	24
External programs and Libraries used by the ADF package.....	28
Tcl/Tk.....	28
Tcllib, including tklib (the Tcl standard library).....	29
VTK.....	30
BLAS.....	31
LAPACK.....	31
ScaLAPACK.....	32
Python 2.7.....	33
Numpy.....	33
SciPy.....	34
Open MPI.....	35
Platform MPI 7.....	37
OpenBabel.....	37
ASE.....	37
PLUMED.....	38
Packmol.....	39
Symmol.....	39
MEAD.....	40
Swish-e.....	40
FFTW.....	40
XCFun.....	40
XQuartz.....	41
RDKit.....	41
PRIMME library.....	42
Eigen library.....	43
PIL.....	43
Boost Library.....	44

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:

1. G. te Velde, F.M. Bickelhaupt, E.J. Baerends, C. Fonseca Guerra, S.J.A. van Gisbergen, 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. ADF2014, 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, H. van Schoot, 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. Wiesenecker, 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 2014:

1. G. te Velde and E.J. Baerends, *Precise density-functional method for periodic structures*, [Physical Review B](#) **44**, 7888 (1991)
2. G. Wiesenecker and E.J. Baerends, *Quadratic integration over the three-dimensional Brillouin zone*, [Journal of Physics: Condensed Matter](#) **3**, 6721 (1991)
3. M. Franchini, P.H.T. Philipsen, L. Visscher, *The Becke Fuzzy Cells Integration Scheme in the Amsterdam Density Functional Program Suite*, [Journal of Computational Chemistry](#) **34**, 1818 (2013).

4. M. Franchini, P.H.T. Philipsen, E. van Lenthe, L. Visscher, *Accurate Coulomb Potentials for Periodic and Molecular Systems through Density Fitting*, *Journal of Chemical Theory and Computation* **10**, 1994 (2014).

5. BAND2014, 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, C.J.O. Verzijl, 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 2014, SCM, Amsterdam, The Netherlands, <http://www.scm.com>

COSMO-RS

For calculations with the COSMO-RS program, version 2014:

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. ADF2014 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, R. Xiong, S.I. Sandler, R.I. Burnett

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

R. Xiong, S.I. Sandler, R.I. Burnett, *An improvement to COSMO-SAC for predicting thermodynamic properties*, *Ind. Eng. Chem. Res.* **53**, 8265 (2014)

DFTB

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

1. ADF DFTB 2014, SCM, Theoretical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands, <http://www.scm.com>

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

Alexei Yakovlev, Pier Philipsen, Stefano Borini, Robert Rürger, Michiel de Reus, Mahdi Ghorbani Asl, Drew McCormack, Serguei Patchkovskii, Thomas Heine

For TD-DFTB, cite:

R. Rürger, E. van Lenthe, Y. Lu, J. Frenzel, T. Heine, and L. Visscher, *Efficient Calculation of Electronic*

Absorption Spectra by Means of Intensity-Selected TD-DFTB, J. Chem. Theory Comp., submitted.
Manuscript available on [arXiv](#).

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 2014, 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, 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
2. J.J.P. Stewart, *Optimization of parameters for semiempirical methods VI: more modifications to the NDDO approximations and re-optimization of parameters*, [J. Mol. Model.](#) **19**, 1-32 (2013)
For parallel calculations, cite:
3. J.D.C. Maia, G.A.U. Carvalho, C.P. Manguiera, S.R. Santana, L.A.F. Cabral, and G.B. Rocha, *GPU Linear Algebra Libraries and GPGPU Programming for Accelerating MOPAC Semiempirical Quantum Chemistry Calculations*, [J. Chem. Theory Comp.](#) **8**, 3072-3081 (2012)

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 2014, 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. Touthkine, 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. Touthkine, 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. Ducéré and L. Cavallo, *Parametrization of an Empirical Correction Term to Density Functional Theory for an Accurate Description of π -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)

J. Autschbach, S. Patchkovskii, T. Ziegler, S.J.A. van Gisbergen and E.J. Baerends, *Chiroptical properties from time-dependent density functional theory. II. Optical rotations of small to medium sized organic molecules*, [Journal of Chemical Physics](#) **117**, 581 (2002)

Magnetizability

Lead

M. Krykunov and J. Autschbach, *Calculation of static and dynamic linear magnetic response in approximate time-dependent density functional theory*, [Journal of Chemical Physics](#) **126**, 24101 (2007)

Magnetic Circular Dichroism (MCD)

M. Seth, M. Krykunov, T. Ziegler, J. Autschbach and A. Banerjee, *Application of magnetically perturbed time-dependent density functional theory to magnetic circular dichroism: Calculation of B terms*, [Journal of Chemical Physics](#) **128**, 144105 (2008)

M. Seth, M. Krykunov, T. Ziegler and J. Autschbach, *Application of magnetically perturbed time-dependent density functional theory to magnetic circular dichroism. II. Calculation of A terms*, [Journal of Chemical Physics](#) **128**, 234102 (2008)

M. Seth, T. Ziegler and J. Autschbach, *Application of magnetically perturbed time-dependent density functional theory to magnetic circular dichroism. III. Temperature-dependent magnetic circular dichroism induced by spin-orbit coupling*, [Journal of Chemical Physics](#) **129**, 104105 (2008)

Verdet constant and Faraday term

M. Krykunov, A. Banerjee, T. Ziegler and J. Autschbach, *Calculation of Verdet constants with time-dependent density functional theory. Implementation and results for small molecules*, [Journal of Chemical Physics](#) **122**, 074105 (2005)

M. Krykunov, M. Seth, T. Ziegler and J. Autschbach, *Calculation of the magnetic circular dichroism B term from the imaginary part of the Verdet constant using damped time-dependent density functional theory*, [Journal of Chemical Physics](#) **127**, 244102 (2007)

NMR

NMR Chemical Shifts

Lead reference

G. Schreckenbach and T. Ziegler, *The calculation of NMR shielding tensors using GIAO's and modern density functional theory*, [Journal of Physical Chemistry](#) **99**, 606 (1995)

NMR chemical shifts with hybrid functionals

M. Krykunov, T. Ziegler and E. van Lenthe, *Hybrid density functional calculations of nuclear magnetic shieldings using Slater-type orbitals and the zeroth-order regular approximation*, [International Journal of Quantum Chemistry](#) **109**, 1676 (2009)

NMR chemical shifts with NBO analysis

J. Autschbach and S. Zheng, *Analyzing Pt chemical shifts calculated from relativistic density functional theory using localized orbitals: The role of Pt 5d lone pairs*, [Magnetic Resonance in Chemistry](#) **46**, S45 (2008)

J. Autschbach, *Analyzing NMR shielding tensors calculated with two-component relativistic methods using spin-free localized molecular orbitals*, [Journal of Chemical Physics](#) **128**, 164112 (2008)

Paramagnetic NMR chemical shifts

J. Autschbach, S. Patchkovskii, and B. Pritchard, *Calculation of Hyperfine Tensors and Paramagnetic NMR Shifts Using the Relativistic Zeroth-Order Regular Approximation and Density Functional Theory*, [Journal of Chemical Theory and Computation](#) **7**, 2175 (2011)

Suggested

G. Schreckenbach and T. Ziegler, *The calculation of NMR shielding tensors based on density functional theory and the frozen-core approximation*, [International Journal of Quantum Chemistry](#) **60**, 753 (1996)

G. Schreckenbach and T. Ziegler, *Calculation of NMR shielding tensors based on density functional theory and a scalar relativistic Pauli-type Hamiltonian. The application to transition metal complexes*, [International Journal of Quantum Chemistry](#) **61**, 899 (1997)

S.K. Wolff and T. Ziegler, *Calculation of DFT-GIAO NMR shifts with inclusion of spin-orbit coupling*, [Journal of Chemical Physics](#) **109**, 895 (1998)

S.K. Wolff, T. Ziegler, E. van Lenthe and E.J. Baerends, *Density functional calculations of nuclear magnetic shieldings using the zeroth-order regular approximation (ZORA) for relativistic effects: ZORA nuclear magnetic resonance*, [Journal of Chemical Physics](#) **110**, 7689 (1999)

NMR spin-spin coupling

Lead

J. Autschbach and T. Ziegler, *Nuclear spin-spin coupling constants from regular approximate density functional calculations. I. Formalism and scalar relativistic results for heavy metal compounds*, [Journal of Chemical Physics](#) **113**, 936 (2000)

J. Autschbach, and T. Ziegler, *Nuclear spin-spin coupling constants from regular approximate relativistic density functional calculations. II. Spin-orbit coupling effects and anisotropies*, [Journal of Chemical Physics](#) **113**, 9410 (2000)

NMR spin-spin couplings with PBE0

J. Autschbach, *Two-component relativistic hybrid density functional computations of nuclear spin-spin coupling tensors using Slater-type basis sets and density-fitting techniques*, [Journal of Chemical Physics](#) **129**, 094105 (2008), Erratum: [Journal of Chemical Physics](#) **130**, 209901 (2009)

NMR spin-spin couplings with NBO analysis

J. Autschbach, *Analyzing molecular properties calculated with two-component relativistic methods using spin-free Natural Bond Orbitals: NMR spin-spin coupling constants* [Journal of Chemical Physics](#) **127**, 124106 (2007)

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)

J. Khandogin and T. Ziegler, *A density functional study of nuclear magnetic resonance spin-spin coupling constants in transition-metal systems*, [Spectrochimica Acta](#) **55**, 607 (1999)

J. Autschbach and T. Ziegler, *Solvent Effects on Heavy Atom Nuclear Spin-Spin Coupling Constants: A Theoretical Study of Hg.C and Pt.P Couplings*, [Journal of the American Chemical Society](#) **123**, 3341 (2001)

J. Autschbach and T. Ziegler, *A Theoretical Investigation of the Remarkable Nuclear Spin-Spin Coupling Pattern in [(NC)₅Pt-Tl(CN)]*, [Journal of the American Chemical Society](#) **123**, 5320 (2001)

Suggested book reference

J. Autschbach, T. Ziegler, in *Encyclopedia of Nuclear Magnetic Resonance*, Eds. D.M. Grant, R. K. Harris, John Wiley and Sons, Chichester, 2002, Vol. 9 *Advances in NMR*.

ESR/EPR

G-tensor: Zeeman interaction

Lead reference (self-consistent spin-orbit coupling)

E. van Lenthe, A. van der Avoird and P.E.S. Wormer, *Density functional calculations of molecular g-tensors in the zero order regular approximation for relativistic effects*, [Journal of Chemical Physics](#) **107**, 2488 (1997)

Lead reference (perturbative inclusion spin-orbit coupling)

J. Autschbach and B. Pritchard, *Calculation of molecular g-tensors using the zeroth-order regular approximation and density functional theory: expectation value versus linear response approaches*, [Theoretical Chemistry Accounts](#) **129**, 453 (2011)

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

G. Schreckenbach and T. Ziegler, *Calculation of the G-tensor of electron paramagnetic resonance spectroscopy using Gauge-Including Atomic Orbitals and Density Functional Theory*, [Journal of Physical Chemistry A](#) **101**, 3388 (1997) (for ESR/EPR g-tensor)

S. Patchkovskii and T. Ziegler, *Calculation of the EPR g-Tensors of High-Spin Radicals with Density Functional Theory*, [Journal of Physical Chemistry A](#) **105**, 5490 (2001) (for high-spin ESR/EPR g-tensor)

A-tensor: Nuclear magnetic dipole hyperfine interaction

Lead reference

E. van Lenthe, A. van der Avoird and P.E.S. Wormer, *Density functional calculations of molecular hyperfine interactions in the zero order regular approximation for relativistic effects*, [Journal of Chemical Physics](#) **108**, 4783 (1998)

Lead reference (perturbative inclusion spin-orbit coupling)

J. Autschbach, S. Patchkovskii, and B. Pritchard, *Calculation of Hyperfine Tensors and Paramagnetic NMR Shifts Using the Relativistic Zeroth-Order Regular Approximation and Density Functional Theory*, [Journal of Chemical Theory and Computation](#) **7**, 2175 (2011)

Electric Field Gradient, NQCC

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

E. van Lenthe and E.J. Baerends, *Density functional calculations of nuclear quadrupole coupling constants in the zero-order regular approximation for relativistic effects*, [Journal of Chemical Physics](#) **112**, 8279 (2000)

EFG with NBO analysis

A.J. Rossini, R.W. Mills, G.A. Briscoe, E.L. Norton, S.J. Geier, I. Hung, S. Zheng, J. Autschbach, and R.W. Schurko, *Solid-State Chlorine NMR of Group IV Transition Metal Organometallic Complexes*, [Journal of the American Chemical Society](#) **131**, 3317 (2009)

J. Autschbach, S. Zheng, and R.W. Schurko, *Analysis of Electric Field Gradient Tensors at Quadrupolar Nuclei in Common Structural Motifs*, [Concepts in Magnetic Resonance Part A](#) **36A**, 84 (2010)

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

Chapter 2 and appendix C of
J.S. Seldenthuis, *Electrical and mechanical effects in single-molecule junctions*, PhD thesis, Delft University of Technology, 2011

Wide-band limit

C.J.O. Verzijl, J.S. Seldenthuis, and J.M. Thijssen, *Applicability of the wide-band limit in DFT-based molecular transport calculations*, [Journal of Chemical Physics](#) **138**, 094102 (2013)

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)

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)

F.M. Bickelhaupt and E.J. Baerends, In: *Rev. Comput. Chem.*; K.B. Lipkowitz and D.B. Boyd, Eds.; Wiley, New York, 2000, Vol. 15, p.1-86

ETS-NOCV

M. Mitoraj, A. Michalak and T. Ziegler, *A Combined Charge and Energy Decomposition Scheme for Bond Analysis*, [Journal of Chemical Theory and Computation](#) **5**, 962 (2009)

QTAIM, Bader analysis

Grid-based algorithm

J.I. Rodríguez, R.F.W. Bader, P.W. Ayers, C. Michel, A.W. Götz and C. Bo, *A high performance grid-based algorithm for computing QTAIM properties*, [Chemical Physics Letters](#) **472**, 149 (2009)

J.I. Rodríguez, *An Efficient Method for Computing the QTAIM Topology of a Scalar Field: The Electron Density Case*, [Journal of Computational Chemistry](#) **34**, 681 (2013)

Accuracy and efficiency

Numerical integration

M. Franchini, P.H.T. Philipsen, L. Visscher, *The Becke Fuzzy Cells Integration Scheme in the Amsterdam Density Functional Program Suite*, [Journal of Computational Chemistry](#) **34**, 1818 (2013).

Density fitting

M. Franchini, P.H.T. Philipsen, E. van Lenthe, L. Visscher, *Accurate Coulomb Potentials for Periodic and Molecular Systems through Density Fitting*, [Journal of Chemical Theory and Computation](#) **10**, 1994 (2014)

Feature References BAND

Lead

See key references above, for all work with BAND

Suggested

G. Wiesenekker, G. te Velde and E.J. Baerends, *Analytic quadratic integration over the two-dimensional Brillouin zone*, [Journal of Physics C: Solid State Physics](#) **21**, 4263 (1988)

G. te Velde and E.J. Baerends, *Numerical integration for polyatomic systems*, [Journal of Computational Physics](#) **99**, 84 (1992)

Geometry optimization

Lead

E.S. Kadantsev, R. Klooster, P.L. de Boeij and T. Ziegler, *The Formulation and Implementation of Analytic Energy Gradients for Periodic Density Functional Calculations with STO/NAO Bloch Basis Set*, [Molecular Physics](#) **105**, 2583 (2007)

TDDFT

Lead

F. Kootstra, P.L. de Boeij and J.G. Snijders, *Efficient real-space approach to time-dependent density functional theory for the dielectric response of nonmetallic crystals*, [Journal of Chemical Physics](#) **112**, 6517 (2000)

P. Romaniello and P.L. de Boeij, *Time-dependent current-density-functional theory for the metallic response of solids*, [Physical Review B](#) **71**, 155108 (2005)

Main applications

F. Kootstra, P.L. de Boeij, and J.G. Snijders, *Application of time-dependent density-functional theory to the dielectric function of various nonmetallic crystals*, [Physical Review B](#) **62**, 7071 (2000)

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

F. Kootstra, [Ph.D. thesis](#), Rijksuniversiteit Groningen, Groningen (2001).

P. Romaniello, [Ph.D. thesis](#), Rijksuniversiteit Groningen, Groningen (2006).

A. Berger, [Ph.D. thesis](#), Rijksuniversiteit Groningen, Groningen (2006).

Relativistic TDDFT

P. Romaniello and P.L. de Boeij, *Relativistic two-component formulation of time-dependent current-density functional theory: Application to the linear response of solids*, [Journal of Chemical Physics](#) **127**, 174111 (2007)

Vignale Kohn

Lead

J.A. Berger, P.L. de Boeij and R. van Leeuwen, *Analysis of the viscoelastic coefficients in the Vignale-Kohn functional: The cases of one- and three-dimensional polyacetylene*, [Physical Review B](#) **71**, 155104 (2005)

Applications

J.A. Berger, P. Romaniello, R. van Leeuwen and P.L. de Boeij, *Performance of the Vignale-Kohn functional in the linear response of metals*, [Physical Review B](#) **74**, 245117 (2006)

J.A. Berger, P.L. de Boeij, and R. van Leeuwen, *Analysis of the Vignale-Kohn current functional in the calculation of the optical spectra of semiconductors*, [Physical Review B](#) **75**, 35116 (2007)

NMR

Lead

D. Skachkov, M. Krykunov, E. Kadantsev, and T. Ziegler, *The Calculation of NMR Chemical Shifts in Periodic Systems Based on Gauge Including Atomic Orbitals and Density Functional Theory*, [Journal of Chemical Theory and Computation](#) **6**, 1650 (2010)

D. Skachkov, M. Krykunov, and T. Ziegler, *An improved scheme for the calculation of NMR chemical shifts in periodic systems based on gauge including atomic orbitals and density functional theory*, [Canadian Journal of Chemistry](#) **89**, 1150 (2011).

ESR

A-tensor: Nuclear magnetic dipole hyperfine interaction

E.S. Kadantsev and T. Ziegler, *Implementation of a Density Functional Theory-Based Method for the Calculation of the Hyperfine A-tensor in Periodic Systems with the Use of Numerical and Slater Type Atomic Orbitals: Application to Paramagnetic Defects*, [Journal of Physical Chemistry A](#) **112**, 4521 (2008)

G-tensor: Zeeman interaction

E.S. Kadantsev and T. Ziegler, *Implementation of a DFT Based Method for the Calculation of Zeeman g-tensor in Periodic Systems with the use of Numerical and Slater Type Atomic Orbitals*, [Journal of Physical Chemistry A](#) **113**, 1327 (2009)

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)

M. J. Mees, G. Pourtois, E. C. Neyts, B. J. Thijsse, A. Stesmans, *Uniform-acceptance force-bias Monte Carlo method with time scale to study solid-state diffusion*, [Physical Review B](#) **85**, 134301 (2012)

Grand Canonical Monte Carlo (GCMC)

Thomas P. Senftle, Randall J. Meyer, Michael J. Janik and Adri C.T. van Duin, *Development of a ReaxFF potential for Pd/O and application to palladium oxide formation*, [J. Chem. Phys.](#) **139**, 044109 (2013)

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)

E. Iype, M. Huetter, A.P.J. Jansen, S.V. Nedeia, C.C.M. Rindt, *Parameterization of a Reactive Force Field Using a Monte Carlo Algorithm*, [J. Comp. Chem.](#) **34**, 1143-1154 (2013)

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

M. Wahiduzzaman, A.F. Oliveira, P.H.T. Philipsen, L. Zhechkov, E. van Lenthe, H.A. Witek, T. Heine, *DFTB Parameters for the Periodic Table: Part 1, Electronic Structure*, [Journal of Chemical Theory and Computation](#) **9**, 4006 (2013)

mio-0-1 from [DFTB.org](#)

For systems containing O, N, C, H:

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)

For systems also containing S:

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

mio-1-1 from [DFTB.org](#)

For systems containing O, N, C, H:

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)

For systems also containing S:

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

For systems also containing P:

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)

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:

S.I. Simdyankin, S.R. Elliott, T.A. Niehaus, and T. Frauenheim, in *Computational Modeling and Simulation of Materials III, vol. A*, P. Vincenzini, A. Lami, F. Zerbetto, Eds.; [Techna Group s.r.l., Faenza, Italy](#), **2004**, pp. 149

matsci-0-3 from [DFTB.org](#) (same origin as Dresden parameters)

The complete set:

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**

For systems containing Al, O, and H:

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)

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

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)

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

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)

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

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)

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

A. Enyashin, J. Frenzel, S. Gemming, G. Seifert *Adsorption of nucleotides on the rutile (110) surface*, *Int. J. Mat. Res.* **101**, 768-764 (2010)

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

N. Jardillier, *Ph.D. Thesis*, Universite Montpellier II, Montpellier (2006)

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:

A. Bondar, S. Fischer, J. C. Smith, M. Elstner, S. Suhai, *Key Role of Electrostatic Interactions in Bacteriorhodopsin Proton Transfer*, *J. Am. Chem. Soc.* **126**, 14668-14677 (2004)

pbcc-0-3 from DFTB.org

For systems containing Si:

A. Sieck, *Ph.D. Thesis*, University of Paderborn, Paderborn (2000).

For systems containing Si and C:

E. Rauls, R. Gutierrez, J. Elsner, Th. Frauenheim, *Stoichiometric and non-stoichiometric (1010) and (1120) surfaces in 2H-SiC: a theoretical study*, *Sol. State Comm.* **111**, 459-464 (1999)

For systems containing Si and O:

C. Koehler, Z. Hajnal, P. Deak, Th. Frauenheim, S. Suhai, *Theoretical investigation of carbon defects and diffusion in alpha-quartz*, *Phys. Rev. B* **64**, 085333 (2001)

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

C. Koehler, Th. Frauenheim, *Molecular dynamics simulations of CF_x (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):

C. Koehler, G. Seifert, Th. Frauenheim *Density functional based calculations for Fe_n (n ≤ 32)*, *Chem. Phys.* **309**, 23-31 (2005)

tiorg-0-1 from DFTB.org

In addition to the mio set, cite:

G. Dolgonos, B. Aradi, N. H. Moreira, Th. Frauenheim, *An Improved Self-Consistent-Charge Density-Functional Tight-Binding (SCC-DFTB) Set of Parameters for Simulation of Bulk and Molecular Systems Involving Titanium*, *J. Chem. Theory Comput.* **6**, 266-278 (2010)

trans3d-0-1 from DFTB.org

In addition to the mio set, cite:

G. Zheng, H. A. Witek, P. Bobadova-Parvanova, S. Irle, D. G. Musaev, R. Prabhakar, K. Morokuma, M. Lundberg, M. Elstner, C. Kohler, T. Frauenheim, *Parameter Calibration of Transition-Metal Elements for the Spin-Polarized Self-Consistent-Charge Density-Functional Tight-Binding (DFTB) Method: Sc, Ti, Fe, Co, and Ni*, *J. Chem. Theory Comput.* **4**, 1349-1367 (2007)

znorg-0-1 from DFTB.org

In addition to the mio set, cite:

N.H. Moreira, G. Dolgonos, B. Aradi, A. L. da Rosa, Th. Frauenheim, *Toward an Accurate Density-Functional Tight-Binding Description of Zinc-Containing Compounds*, *J. Chem. Theory Comput.* **4**, 605-614 (2009)

3ob-1-1 from DFTB.org

For systems containing O, N, C, H:

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

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/>

License:

BSD-style open source license

This software is copyrighted by the Regents of the University of California, Sun Microsystems, Inc., Scriptics Corporation, ActiveState Corporation and other parties. The following terms apply to all files associated with the software unless explicitly disclaimed in individual files.

The authors hereby grant permission to use, copy, modify, distribute, and license this software and its documentation for any purpose, provided that existing copyright notices are retained in all copies and that this notice is included verbatim in any distributions. No written agreement, license, or royalty fee is required for any of the authorized uses. Modifications to this software may be copyrighted by their authors and need not follow the licensing terms described here, provided that the new terms are clearly indicated on the first page of each file where they apply.

IN NO EVENT SHALL THE AUTHORS OR DISTRIBUTORS BE LIABLE TO ANY PARTY FOR DIRECT, INDIRECT, SPECIAL, INCIDENTAL, OR CONSEQUENTIAL DAMAGES ARISING OUT OF THE USE OF THIS SOFTWARE, ITS DOCUMENTATION, OR ANY DERIVATIVES THEREOF, EVEN IF THE AUTHORS HAVE BEEN ADVISED OF THE POSSIBILITY OF SUCH DAMAGE.

THE AUTHORS AND DISTRIBUTORS SPECIFICALLY DISCLAIM ANY WARRANTIES, INCLUDING, BUT NOT LIMITED TO, THE IMPLIED WARRANTIES OF MERCHANTABILITY, FITNESS FOR A PARTICULAR PURPOSE, AND NON-INFRINGEMENT. THIS SOFTWARE IS PROVIDED ON AN "AS IS" BASIS, AND THE AUTHORS AND DISTRIBUTORS HAVE NO OBLIGATION TO PROVIDE MAINTENANCE, SUPPORT, UPDATES, ENHANCEMENTS, OR MODIFICATIONS.

GOVERNMENT USE: If you are acquiring this software on behalf of the U.S. government, the Government shall have only "Restricted Rights" in the software and related documentation as defined in the Federal Acquisition Regulations (FARs) in Clause 52.227.19 (c) (2). If you are acquiring the software on behalf of the Department of Defense, the

software shall be classified as "Commercial Computer Software" and the Government shall have only "Restricted Rights" as defined in Clause 252.227-7013 (b) (3) of DFARs. Notwithstanding the foregoing, the authors grant the U.S. Government and others acting in its behalf permission to use and distribute the software in accordance with the terms specified in this license.

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:

This software is copyrighted by Ajuba Solutions and other parties. The following terms apply to all files associated with the software unless explicitly disclaimed in individual files.

The authors hereby grant permission to use, copy, modify, distribute, and license this software and its documentation for any purpose, provided that existing copyright notices are retained in all copies and that this notice is included verbatim in any distributions. No written agreement, license, or royalty fee is required for any of the authorized uses. Modifications to this software may be copyrighted by their authors and need not follow the licensing terms described here, provided that the new terms are clearly indicated on the first page of each file where they apply.

IN NO EVENT SHALL THE AUTHORS OR DISTRIBUTORS BE LIABLE TO ANY PARTY FOR DIRECT, INDIRECT, SPECIAL, INCIDENTAL, OR CONSEQUENTIAL DAMAGES ARISING OUT OF THE USE OF THIS SOFTWARE, ITS DOCUMENTATION, OR ANY DERIVATIVES THEREOF, EVEN IF THE AUTHORS HAVE BEEN ADVISED OF THE POSSIBILITY OF SUCH DAMAGE.

THE AUTHORS AND DISTRIBUTORS SPECIFICALLY DISCLAIM ANY WARRANTIES, INCLUDING, BUT NOT LIMITED TO, THE IMPLIED WARRANTIES OF MERCHANTABILITY, FITNESS FOR A PARTICULAR PURPOSE, AND NON-INFRINGEMENT. THIS SOFTWARE IS PROVIDED ON AN "AS IS" BASIS, AND THE AUTHORS AND DISTRIBUTORS HAVE NO OBLIGATION TO PROVIDE MAINTENANCE, SUPPORT, UPDATES, ENHANCEMENTS, OR

MODIFICATIONS.

GOVERNMENT USE: If you are acquiring this software on behalf of the U.S. government, the Government shall have only "Restricted Rights" in the software and related documentation as defined in the Federal Acquisition Regulations (FARs) in Clause 52.227.19 (c) (2). If you are acquiring the software on behalf of the Department of Defense, the software shall be classified as "Commercial Computer Software" and the Government shall have only "Restricted Rights" as defined in Clause 252.227-7013 (c) (1) of DFARs. Notwithstanding the foregoing, the authors grant the U.S. Government and others acting in its behalf permission to use and distribute the software in accordance with the terms specified in this license.

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
All rights reserved.

Redistribution and use in source and binary forms, with or without modification, are permitted provided that the following conditions are met:

- Redistributions of source code must retain the above copyright notice, this list of conditions and the following disclaimer.
- Redistributions in binary form must reproduce the above copyright notice, this list of conditions and the following disclaimer in the documentation and/or other materials provided with the distribution.
- Neither name of Ken Martin, Will Schroeder, or Bill Lorensen nor the names of any contributors may be used to endorse or promote products derived from this software without specific prior written permission.

THIS SOFTWARE IS PROVIDED BY THE COPYRIGHT HOLDERS AND CONTRIBUTORS "AS IS" AND ANY EXPRESS OR IMPLIED WARRANTIES, INCLUDING, BUT NOT LIMITED TO, THE IMPLIED WARRANTIES OF MERCHANTABILITY AND FITNESS FOR A PARTICULAR PURPOSE ARE DISCLAIMED. IN NO EVENT SHALL THE AUTHORS OR CONTRIBUTORS BE LIABLE FOR ANY DIRECT, INDIRECT, INCIDENTAL, SPECIAL, EXEMPLARY, OR CONSEQUENTIAL DAMAGES (INCLUDING, BUT NOT LIMITED TO, PROCUREMENT OF SUBSTITUTE GOODS OR SERVICES; LOSS OF USE, DATA, OR PROFITS; OR BUSINESS INTERRUPTION) HOWEVER CAUSED AND ON ANY THEORY OF LIABILITY, WHETHER IN CONTRACT, STRICT LIABILITY, OR TORT (INCLUDING NEGLIGENCE OR OTHERWISE) ARISING IN ANY WAY OUT OF THE USE OF THIS SOFTWARE, EVEN IF ADVISED OF THE POSSIBILITY OF SUCH DAMAGE.

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

Copyright (c) 1992-2010 The University of Tennessee and The University of Tennessee Research Foundation. All rights reserved.

Copyright (c) 2000-2010 The University of California Berkeley. All rights reserved.

Copyright (c) 2006-2010 The University of Colorado Denver. All rights reserved.

\$COPYRIGHT\$

Additional copyrights may follow

\$HEADER\$

Redistribution and use in source and binary forms, with or without modification, are permitted provided that the following conditions are met:

- Redistributions of source code must retain the above copyright notice, this list of conditions and the following disclaimer.
- Redistributions in binary form must reproduce the above copyright notice, this list of conditions and the following disclaimer listed in this license in the documentation and/or other materials provided with the distribution.
- Neither the name of the copyright holders nor the names of its contributors may be used to endorse or promote products derived from this software without specific prior written permission.

The copyright holders provide no reassurances that the source code provided does not infringe any patent, copyright, or any other intellectual property rights of third parties. The copyright holders disclaim any liability to any recipient for claims brought against recipient by any third party for infringement of that parties intellectual property rights.

THIS SOFTWARE IS PROVIDED BY THE COPYRIGHT HOLDERS AND CONTRIBUTORS "AS IS" AND ANY EXPRESS OR IMPLIED WARRANTIES, INCLUDING, BUT NOT LIMITED TO, THE 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, EXEMPLARY, OR CONSEQUENTIAL DAMAGES (INCLUDING, BUT NOT LIMITED TO, PROCUREMENT OF SUBSTITUTE GOODS OR SERVICES; LOSS OF USE, DATA, OR PROFITS; OR BUSINESS INTERRUPTION) HOWEVER CAUSED AND ON ANY THEORY OF LIABILITY, WHETHER IN CONTRACT, STRICT LIABILITY, OR TORT (INCLUDING NEGLIGENCE OR OTHERWISE) ARISING IN ANY WAY OUT OF THE USE OF THIS SOFTWARE, EVEN IF ADVISED OF THE POSSIBILITY OF SUCH DAMAGE.

ScaLAPACK

Description:

implementation of a subset of LAPACK routines for parallel computers

Site:

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

License:

modified BSD

Copyright (c) 1992-2009 The University of Tennessee. All rights reserved.

\$COPYRIGHT\$

Additional copyrights may follow

\$HEADER\$

Redistribution and use in source and binary forms, with or without modification, are permitted provided that the following conditions are met:

- Redistributions of source code must retain the above copyright notice, this list of conditions and the following disclaimer.
- Redistributions in binary form must reproduce the above copyright notice, this list of conditions and the following disclaimer listed in this license in the documentation and/or other materials provided with the distribution.
- Neither the name of the copyright holders nor the names of its contributors may be used to endorse or promote products derived from this software without specific prior written permission.

THIS SOFTWARE IS PROVIDED BY THE COPYRIGHT HOLDERS AND CONTRIBUTORS "AS IS" AND ANY EXPRESS OR IMPLIED WARRANTIES, INCLUDING, BUT NOT LIMITED TO, THE 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, EXEMPLARY, OR CONSEQUENTIAL DAMAGES (INCLUDING, BUT NOT LIMITED TO, PROCUREMENT OF SUBSTITUTE GOODS OR SERVICES; LOSS OF USE, DATA, OR PROFITS; OR BUSINESS INTERRUPTION) HOWEVER CAUSED AND ON ANY THEORY OF LIABILITY, WHETHER IN CONTRACT, STRICT LIABILITY, OR TORT (INCLUDING NEGLIGENCE OR OTHERWISE) ARISING IN ANY WAY OUT OF THE USE OF THIS SOFTWARE, EVEN IF ADVISED OF THE POSSIBILITY OF SUCH DAMAGE.

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
Copyright (c) 2005-2011, NumPy Developers.
All rights reserved.

Redistribution and use in source and binary forms, with or without modification, are permitted provided that the following conditions are met:

- * Redistributions of source code must retain the above copyright notice, this list of conditions and the following disclaimer.
- * Redistributions in binary form must reproduce the above copyright notice, this list of conditions and the following disclaimer in the documentation and/or other materials provided with the distribution.
- * Neither the name of the NumPy Developers nor the names of any contributors may be used to endorse or promote products derived from this software without specific prior written permission.

THIS SOFTWARE IS PROVIDED BY THE COPYRIGHT HOLDERS AND CONTRIBUTORS "AS IS" AND ANY EXPRESS OR IMPLIED WARRANTIES, INCLUDING, BUT NOT LIMITED TO, THE 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, EXEMPLARY, OR CONSEQUENTIAL DAMAGES (INCLUDING, BUT NOT LIMITED TO, PROCUREMENT OF SUBSTITUTE GOODS OR SERVICES; LOSS OF USE, DATA, OR PROFITS; OR BUSINESS INTERRUPTION) HOWEVER CAUSED AND ON ANY THEORY OF LIABILITY, WHETHER IN CONTRACT, STRICT LIABILITY, OR TORT (INCLUDING NEGLIGENCE OR OTHERWISE) ARISING IN ANY WAY OUT OF THE USE OF THIS SOFTWARE, EVEN IF ADVISED OF THE POSSIBILITY OF SUCH DAMAGE.

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.

Copyright (c) 2003-2012 SciPy Developers.
All rights reserved.

Redistribution and use in source and binary forms, with or without modification, are permitted provided that the following conditions are met:

- a. Redistributions of source code must retain the above copyright notice, this list of conditions and the following disclaimer.
- b. Redistributions in binary form must reproduce the above copyright notice, this list of conditions and the following disclaimer in the documentation and/or other materials provided with the distribution.
- c. Neither the name of Enthought nor the names of the SciPy Developers may be used to endorse or promote products derived from this software without specific prior written permission.

THIS SOFTWARE IS PROVIDED BY THE COPYRIGHT HOLDERS AND CONTRIBUTORS "AS IS"

AND ANY EXPRESS OR IMPLIED WARRANTIES, INCLUDING, BUT NOT LIMITED TO, THE IMPLIED WARRANTIES OF MERCHANTABILITY AND FITNESS FOR A PARTICULAR PURPOSE

ARE DISCLAIMED. IN NO EVENT SHALL THE COPYRIGHT HOLDERS OR CONTRIBUTORS BE LIABLE FOR ANY DIRECT, INDIRECT, INCIDENTAL, SPECIAL, EXEMPLARY, OR CONSEQUENTIAL DAMAGES (INCLUDING, BUT NOT LIMITED TO, PROCUREMENT OF SUBSTITUTE GOODS OR SERVICES; LOSS OF USE, DATA, OR PROFITS; OR BUSINESS INTERRUPTION) HOWEVER CAUSED AND ON ANY THEORY OF LIABILITY, WHETHER IN CONTRACT, STRICT LIABILITY, OR TORT (INCLUDING NEGLIGENCE OR OTHERWISE) ARISING IN ANY WAY OUT OF THE USE OF THIS SOFTWARE, EVEN IF ADVISED OF THE POSSIBILITY OF SUCH DAMAGE.

Open MPI

Description:

Open source MPI-2 implementation

Site:

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

License:

New BSD License

Following is the text of the New BSD license, taken from <http://www.open-mpi.org/community/license.php>:

Most files in this release are marked with the copyrights of the organizations who have edited them. The copyrights below are in no particular order and generally reflect members of the Open MPI core team who have contributed code to this release. The copyrights for code used under license from other parties are included in the corresponding files.

Copyright (c) 2004-2010 The Trustees of Indiana University and Indiana University Research and Technology

Corporation. All rights reserved.
Copyright (c) 2004-2010 The University of Tennessee and The University of Tennessee Research Foundation. All rights reserved.
Copyright (c) 2004-2010 High Performance Computing Center Stuttgart, University of Stuttgart. All rights reserved.
Copyright (c) 2004-2008 The Regents of the University of California. All rights reserved.
Copyright (c) 2006-2010 Los Alamos National Security, LLC. All rights reserved.
Copyright (c) 2006-2010 Cisco Systems, Inc. All rights reserved.
Copyright (c) 2006-2010 Voltaire, Inc. All rights reserved.
Copyright (c) 2006-2010 Sandia National Laboratories. All rights reserved.
Copyright (c) 2006-2010 Sun Microsystems, Inc. All rights reserved.
Use is subject to license terms.
Copyright (c) 2006-2010 The University of Houston. All rights reserved.
Copyright (c) 2006-2009 Myricom, Inc. All rights reserved.
Copyright (c) 2007-2008 UT-Battelle, LLC. All rights reserved.
Copyright (c) 2007-2010 IBM Corporation. All rights reserved.
Copyright (c) 1998-2005 Forschungszentrum Juelich, Juelich Supercomputing Centre, Federal Republic of Germany
Copyright (c) 2005-2008 ZIH, TU Dresden, Federal Republic of Germany
Copyright (c) 2007 Evergrid, Inc. All rights reserved.
Copyright (c) 2008 Chelsio, Inc. All rights reserved.
Copyright (c) 2008-2009 Institut National de Recherche en Informatique. All rights reserved.
Copyright (c) 2007 Lawrence Livermore National Security, LLC. All rights reserved.
Copyright (c) 2007-2009 Mellanox Technologies. All rights reserved.
Copyright (c) 2006-2010 QLogic Corporation. All rights reserved.
Copyright (c) 2008-2010 Oak Ridge National Labs. All rights reserved.
Copyright (c) 2006-2010 Oracle and/or its affiliates. All rights reserved.
Copyright (c) 2009 Bull SAS. All rights reserved.
Copyright (c) 2010 ARM Ltd. All rights reserved.

\$COPYRIGHT\$

Additional copyrights may follow

\$HEADER\$

Redistribution and use in source and binary forms, with or without modification, are permitted provided that the following conditions are met:

- Redistributions of source code must retain the above copyright notice, this list of conditions and the following disclaimer.
- Redistributions in binary form must reproduce the above copyright notice, this list of conditions and the following disclaimer listed in this license in the documentation and/or other materials provided with the distribution.
- Neither the name of the copyright holders nor the names of its contributors may be used to endorse or promote products derived from this software without specific prior written permission.

The copyright holders provide no reassurances that the source code provided does not infringe any patent, copyright, or any other intellectual property rights of third parties. The copyright holders disclaim any liability to any recipient for claims brought against recipient by any third party for infringement of that parties intellectual property rights.

THIS SOFTWARE IS PROVIDED BY THE COPYRIGHT HOLDERS AND CONTRIBUTORS "AS IS" AND ANY EXPRESS OR IMPLIED WARRANTIES, INCLUDING, BUT NOT LIMITED TO, THE 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, EXEMPLARY, OR CONSEQUENTIAL DAMAGES (INCLUDING, BUT NOT LIMITED TO, PROCUREMENT OF SUBSTITUTE GOODS OR SERVICES; LOSS OF USE, DATA, OR PROFITS; OR BUSINESS INTERRUPTION) HOWEVER CAUSED AND ON ANY THEORY OF LIABILITY, WHETHER IN CONTRACT, STRICT LIABILITY, OR TORT (INCLUDING NEGLIGENCE OR OTHERWISE) ARISING IN ANY WAY OUT OF THE USE OF THIS SOFTWARE, EVEN IF ADVISED OF THE POSSIBILITY OF SUCH DAMAGE.

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](#)
Comput. Sci. Eng., Vol. **4**, 56-66, 2002

License:

GNU Lesser General Public License version 2.1

LICENSE included in the distribution:

ASE is free software: you can redistribute it and/or modify it under the terms of the GNU Lesser General Public License as published by the Free Software Foundation, either version 2.1 of the License, or (at your option) any later version.

ASE is distributed in the hope that it will be useful, but WITHOUT ANY WARRANTY; without even the implied warranty of MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE. See the GNU Lesser General Public License for more details.

You should have received a copy of the GNU Lesser General Public License along with ASE. If not, see <http://www.gnu.org/licenses/>.

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. Comm. 2009 vol. **180** (10) pp. 1961-1972.

License:

GNU Lesser General Public License version 3

LICENSE included in the distribution:

PLUMED is free software: you can redistribute it and/or modify it under the terms of the GNU Lesser General Public License as published by the Free Software Foundation, either version 3 of the License, or (at your option) any later version.
PLUMED is distributed in the hope that it will be useful, but WITHOUT ANY WARRANTY; without even the implied warranty of MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE. See the GNU Lesser General Public License for more detail.

You should have received a copy of the GNU Lesser General Public License along with PLUMED. If not, see <http://www.gnu.org/licenses/>.

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.
[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.

Site:

<http://swish-e.org/>

License:

a modified version of GNU GPL2

[Click](http://swish-e.org/license.html) 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:

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 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](#). 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:

BSD licensed according to the documentation.

In the README: Please see the file license.txt for details about the "New BSD" license which covers this software and its associated data and documents. The file license.txt has the following contents:

Unless otherwise noted, all files in this directory and all subdirectories are distributed under the following license:

Copyright (c) 2006-2014
Rational Discovery LLC, Greg Landrum, and Julie Penzotti

All rights reserved.

Redistribution and use in source and binary forms, with or without modification, are permitted provided that the following conditions are met:

- * Redistributions of source code must retain the above copyright notice, this list of conditions and the following disclaimer.
- * Redistributions in binary form must reproduce the above copyright notice, this list of conditions and the following disclaimer in the documentation and/or other materials provided with the distribution.
- * Neither the name of Rational Discovery nor the names of its contributors may be used to endorse or promote products derived from this software without specific prior written permission.

THIS SOFTWARE IS PROVIDED BY THE COPYRIGHT HOLDERS AND CONTRIBUTORS "AS IS" AND ANY EXPRESS OR IMPLIED WARRANTIES, INCLUDING, BUT NOT LIMITED TO, THE 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, EXEMPLARY, OR CONSEQUENTIAL DAMAGES (INCLUDING, BUT NOT LIMITED TO, PROCUREMENT OF SUBSTITUTE GOODS OR SERVICES; LOSS OF USE, DATA, OR PROFITS; OR BUSINESS INTERRUPTION) HOWEVER CAUSED AND ON ANY THEORY OF LIABILITY, WHETHER IN CONTRACT, STRICT LIABILITY, OR TORT (INCLUDING NEGLIGENCE OR OTHERWISE) ARISING IN ANY WAY OUT OF THE USE OF THIS SOFTWARE, EVEN IF ADVISED OF THE POSSIBILITY OF SUCH DAMAGE.

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:

Andreas Stathopoulos and James R. McCombs, [PRIMME: PReconditioned Iterative MultiMethod Eigensolver: Methods and software description](#) ACM Transaction on Mathematical Software Vol. 37, No. 2, (2010), 21:1--21:30.

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

By obtaining, using, and/or copying this software and/or its associated documentation, you agree that you have read, understood, and will comply with the following terms and conditions:

Permission to use, copy, modify, and distribute this software and its associated documentation for any purpose and without fee is hereby granted, provided that the above copyright notice appears in all copies, and that both that copyright notice and this permission notice appear in supporting documentation, and that the name of Secret Labs AB or the author not be used in advertising or publicity pertaining to distribution of the software without specific, written prior permission.

SECRET LABS AB AND THE AUTHOR DISCLAIMS ALL WARRANTIES WITH REGARD TO THIS SOFTWARE, INCLUDING ALL IMPLIED WARRANTIES OF MERCHANTABILITY AND FITNESS. IN NO EVENT SHALL SECRET LABS AB OR THE AUTHOR BE LIABLE FOR ANY SPECIAL, INDIRECT OR CONSEQUENTIAL DAMAGES OR ANY DAMAGES WHATSOEVER RESULTING FROM LOSS OF USE, DATA OR PROFITS, WHETHER IN AN ACTION OF CONTRACT, NEGLIGENCE OR OTHER TORTIOUS ACTION, ARISING OUT OF OR IN CONNECTION WITH THE USE OR PERFORMANCE OF THIS SOFTWARE.

Boost Library

Description:

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

Site:

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

License:

Boost Software License - Version 1.0 - August 17th, 2003

Permission is hereby granted, free of charge, to any person or organization obtaining a copy of the software and accompanying documentation covered by this license (the "Software") to use, reproduce, display, distribute, execute, and transmit the Software, and to prepare derivative works of the Software, and to permit third-parties to whom the Software is furnished to do so, all subject to the following:

The copyright notices in the Software and this entire statement, including the above license grant, this restriction and the following disclaimer, must be included in all copies of the Software, in whole or in part, and all derivative works of the Software, unless such copies or derivative works are solely in the form of machine-executable object code generated by a source language processor.

THE SOFTWARE IS PROVIDED "AS IS", WITHOUT WARRANTY OF ANY KIND, EXPRESS OR IMPLIED, INCLUDING BUT NOT LIMITED TO THE WARRANTIES OF MERCHANTABILITY,

FITNESS FOR A PARTICULAR PURPOSE, TITLE AND NON-INFRINGEMENT. IN NO EVENT SHALL THE COPYRIGHT HOLDERS OR ANYONE DISTRIBUTING THE SOFTWARE BE LIABLE FOR ANY DAMAGES OR OTHER LIABILITY, WHETHER IN CONTRACT, TORT OR OTHERWISE, ARISING FROM, OUT OF OR IN CONNECTION WITH THE SOFTWARE OR THE USE OR OTHER DEALINGS IN THE SOFTWARE.