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

Table of Contents

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. 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 2014:

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. 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 Rüger, Michiel de Reus, Mahdi Ghorbani Asl, Drew McCormack, Serguei Patchkovskii, Thomas Heine

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

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. Mangueira, 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* H_2CO, 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 $M(COT)_2$, M=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 Acadamic 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 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 hepta-helicenes*, 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 $M(CO)_6$ (M = Cr, Mo, 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. vand 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 C_{60}*, 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 C_6, C_7, and C_8 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)

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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)

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For systems containing O, N, C, H:
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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)

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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)

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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

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In addition to the mio set, cite:
G. Dolgonos, B. Aradi, N. H. Moreira, T. 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 Compt. **6**, 266-278 (2010)

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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 Compt. **4**, 1349-1367 (2007)

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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)

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External programs and Libraries used by the ADF package

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We will gladly answer any questions regarding the software. If a modification is done, however, it is the responsibility of the person who modified the routine to provide support.

LAPACK

Description:

Linear Algebra library

Site:

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

License:

modified BSD

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ScaLAPACK

Description:

implementation of a subset of LAPACK routines for parallel computers

Site:

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

License:

modified BSD

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Python 2.7

Description:

scripting language

Site:

http://www.python.org/

License:

open source, GPL compatible

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

Numpy

Description:

Libary for scientific computing with Python

Site:

http://www.numpy.org/

License:

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SciPy

Description:

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

Site:

http://scipy.org/scipylib/

License:

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Open MPI

Description:

Open source MPI-2 implementation

Site:

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

License:

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

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:

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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
An object-oriented scripting interface to a legacy electronic structure code
Comput. Sci. Eng., Vol. **4**, 56-66, 2002

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PLUMED

Description:

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

Site:

http://www.plumed-code.org

Reference:

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

Bonomi, D. Branduardi, G. Bussi, C. Camilloni, D. Provasi, P. Raiteri, D. Donadio, F. Marinelli, F. Pietrucci, R.A. Broglia and M. Parrinello
PLUMED: a portable plugin for free-energy calculations with molecular dynamics, Comp. Phys. Comm. 2009 vol. **180** (10) pp. 1961-1972.

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Packmol

Description:

Packing Optimization for Molecular Dynamics Simulations

Packmol (version of november 2009) is used to generate MD starting geometries. No changes have been made to the source code, and the version of the source code that we have used is included in $ADFHOME/Install/packmol.tar (november 2009).

Packmol is executed as an (external) stand-alone command via the GUI.

Site:

http://www.ime.unicamp.br/~martinez/packmol/

License:

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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

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FFTW

Description:

Library to compute the discrete Fourier transform

Site:

http://www.fftw.org/

License:

commercial

XCFun

Description:

XCFun is a library of approximate exchange-correlation functionals

Site:

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

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 aplication 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/

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PRIMME library

Description:

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

Site:

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

Reference:

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:

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The following header is included with the Eigen library:
This file is part of Eigen, a lightweight C++ template library
for linear algebra.
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#
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

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Boost Library

Description:

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

Site:

http://www.boost.org/

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