Scientific Computing & Modelling

References

ADF Program System
Release 2010

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

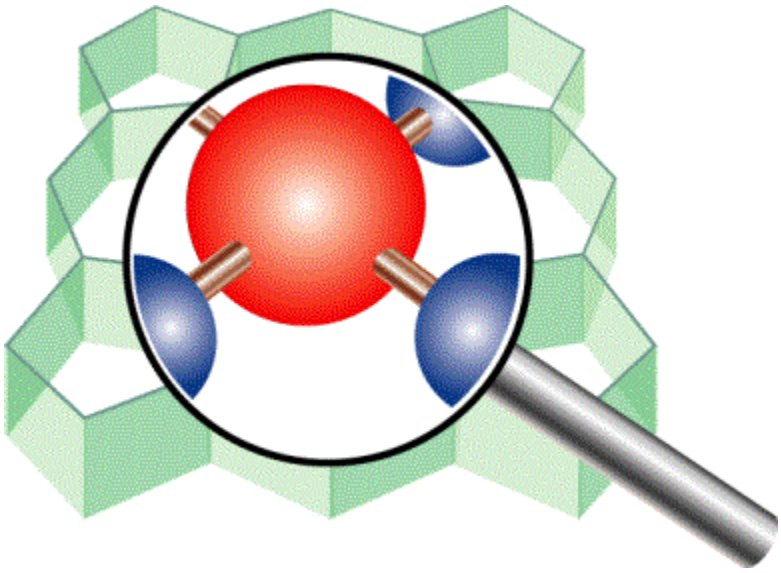

Table of Contents

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 2010:

1. G. te Velde, F.M. Bickelhaupt, S.J.A. van Gisbergen, C. Fonseca Guerra, E.J. Baerends, J.G. Snijders and T. Ziegler, *Chemistry with ADF.* Journal of Compututational 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. ADF2010, 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, 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, J. Neugebauer, V.P. Nicu, L. Noodleman, V.P. Osinga, S. Patchkovskii, P.H.T. Philipsen, D. Post, C.C. Pye, W. Ravenek, J.I. Rodríguez, P. Ros, P.R.T. Schipper, G. Schreckenbach, J.S. Seldenthuis, M. Seth, J.G. Snijders, M. Solà, M. Swart, D. Swerhone, G. te Velde, P. Vernooijs, L. Versluis, L. Visscher, O. Visser, F. Wang, T.A. Wesolowski, E.M. van Wezenbeek, G. Wiesenekker, S.K. Wolff, T.K. Woo, A.L. Yakovlev

Note: if you have used a modified (by yourself, for instance) version of the code, you should mention in the citation that a modified version has been used.

BAND

For calculations with the periodic structures BAND program, version 2010:

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. BAND2010, 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, J.A. Groeneveld, E.S.

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

Note: if you have used a modified (by yourself, for instance) version of the code, you should mention in the citation that a modified version has been used.

COSMO-RS

For calculations with the COSMO-RS program, version 2010:

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. ADF2010 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

ADF-GUI and BAND-GUI

The ADF-GUI and BAND-GUI have been developed within SCM (with O. Visser as primary developer).
Main contributions outside SCM have come from:
P. Leyronnas, W.-J. van Zeist, and M. Luppi.

If you used the ADF-GUI (for example ADFview) you may optionally include the reference:

ADF-GUI 2010, SCM, Amsterdam, The Netherlands, http://www.scm.com

Likewise if you used the BAND-GUI you may optionally include the reference:

BAND-GUI 2010, SCM, Amsterdam, The Netherlands, http://www.scm.com

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 2010, 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

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

The ReaxFF program has been optimized (much faster, running in parallel, and using shared memory) 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 .

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

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)

Quild

For calculations with the Quild program

M. Swart and F.M. Bickelhaupt, *QUILD: QUantum-regions interconnected by local descriptions.* Journal of Compututational Chemistry **29**, 724 (2007)

DFTB

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

1. T. Frauenheim, G. Seifert, M. Elstner, Z. Hajnal, G. Jungnickel, D. Porezag, S. Suhai and R. Scholz, *A Self-Consistent Charge Density-Functional Based Tight-Binding Method for Predictive Materials Simulations in Physics, Chemistry and Biology.* Physica Status Solidi (b) **217**, 41 (2000)

2. ADF2010 DFTB, SCM, Theoretical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands, http://www.scm.com
Optionally, you may add the author: D.A. McCormack

DFTB parameter files available in the ADF package

J. Frenzel, A. F. Oliveira N. Jardillier, T. Heine, and G. Seifert, *Semi-relativistic, self-consistent charge Slater-Koster tables for density-functional based tight-binding (DFTB) for materials science simulations*, TU-Dresden 2004-2010.

Model Hamiltonians

Density Functional

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 Compututational Chemistry **29**, 1011 (2008)

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)

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)

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)

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 $[(NC)_5Pt\text{-}Tl(CN)]^-$.* 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 references (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)

Lead reference (ADF)

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)

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)

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)

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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)

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)

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)

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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)

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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).

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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)

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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)

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)

ReaxFF Force Field References

When you publish results in the scientific literature that were obtained with one of the included force fields for ReaxFF, including the proper reference for the force field used is mandatory.

AB (Ammonia Borane):

> M.R. Weismiller, A.C.T. van Duin, J. Lee, R.A. Yetter, *ReaxFF Reactive Force Field Development and Applications for Molecular Dynamics Simulations of Ammonia Borane Dehydrogenation and Combustion.* Journal of Physical Chemistry A **114**, 5485-5492 (2010)

AuO:

> J.A. Keith, D. Fantauzzi, T. Jacob, A.C.T. van Duin, *Reactive forcefield for simulating gold surfaces and nanoparticles.* Physical Review B **81**, 235404 (2010)

CHO (Hydrocarbon oxidation):

> K. Chenoweth, A.C.T. van Duin, W.A. Goddard, *ReaxFF Reactive Force Field for Molecular Dynamics Simulations of Hydrocarbon Oxidation.* Journal of Physical Chemistry A **112**, 1040-1053 (2008)

Cu-water:

> A.C.T. van Duin, V.S. Bryantsev, M.S. Diallo, W.A. Goddard, O. Rahaman, D.J. Doren, D. Raymand, and K. Hermansson, *Development and validation of a ReaxFF reactive force field for Cu cation/water interactions and copper metal/metal oxide/metal hydroxide condensed phases.* Journal of Physical Chemistry A **114**, 9507-9514 (2010)

FeOCH:

> M. Aryanpour, A.C.T. van Duin, J.D. Kubicki, *Article Development of a Reactive Force Field for Iron.Oxyhydroxide Systems.* Journal of Physical Chemistry A **114**, 6298-6307 (2010)

HE (RDX/High Energy):

> A. Strachan, A.C.T. van Duin, D. Chakraborty, S. Dasgupta, W.A. Goddard III, *Shock Waves in High-Energy Materials: The Initial Chemical Events in Nitramine RDX.* Physical Review Letters **91**, 098301 (2003)
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> A. Strachan, E. Kober, A.C.T. van Duin, J. Oxgaard, W.A. Goddard III, *Thermal decomposition of RDX from reactive molecular dynamics.* Journal of Chemical Physics **122**, 054502 (2005)
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> L. Zhang, S. Zybin, A.C.T. van Duin, S. Dasgupta, W.A. Goddard, E.J. Kober, *Carbon Cluster Formation during Thermal Decomposition of Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine and 1,3,5-Triamino-2,4,6-trinitrobenzene High Explosives from ReaxFF Reactive Molecular Dynamics Simulations.* Journal of Physical Chemistry A **113**, 10619-10640 (2009)

NaH:

> J.G.O. Ojwang, R. Van Santen, G.J. Kramer, A.C.T. van Duin, and W.A. Goddard, *Modeling the sorption dynamics of NaH using a reactive force field.* Journal of Chemical Physics **128**, 164714 (2008)

NiCH:

J.E. Mueller, A.C.T. van Duin, and W.A. Goddard, III, *Development and Validation of ReaxFF Reactive Force Field for Hydrocarbon Chemistry Catalyzed by Nickel.* Journal of Physical Chemistry C **114**, 4939-4949 (2010)

VOCH:

K. Chenoweth, A.C.T. van Duin, P. Persson, M.J. Cheng, J. Oxgaard, W.A. Goddard, *Development and Application of a ReaxFF Reactive Force Field for Oxidative Dehydrogenation on Vanadium Oxide Catalysts.* Journal of Physical Chemistry C **112**, 14645-14654 (2008)

ZnOH:

D. Raymand, A.C.T. van Duin, M. Baudin, K. Hermannson, *A reactive force field (ReaxFF) for zinc oxide.* Surface Science **602** (5), 1020-1031 (2008)

D. Raymand, A.C.T. van Duin, D. Spangberg, W.A. Goddard, K. Hermansson, *Water adsorption on stepped ZnO surfaces from MD simulation.* Surface Science **604** (9-10), 741-752 (2010)

External programs and Libraries used by the ADF package

The next programs and/or libraries are used in the ADF package. On some platforms optimized libraries have been used and/or vendor specific MPI implementations.

Tcl/Tk

Description:

the scripting language used internally within the ADF package

Site:

http://www.tcl.tk/

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Tcllib, including tklib (the Tcl standard library)

Description:

standard library belonging to Tcl/Tk

Site:

http://www.tcl.tk/software/tcllib/

License:

BSD

On the TclTk wiki the following is mentioned about the license:

In response to popular demand, the Tcl core group is introducing tcllib, a Tcl standard library. This meta-package will contain many modules, each of which is itself a standalone Tcl package. The intention is to provide commonly used functions and libraries, bundled together under a single license (BSD), and with no binary dependencies.

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VTK

Description:

the visualization toolkit used by the GUI

Site:

http://www.vtk.org/

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BLAS

Description:

Linear Algebra library

Site:

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

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The following information is from the BLAS FAQ on the mentioned site:

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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.

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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

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Linear Algebra library

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ScaLAPACK

Description:

implementation of a subset of LAPACK routines for parallel computers

Site:

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

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Python 2.6

Description:

scripting language

Site:

http://www.python.org/

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Numpy

Description:

Libary for scientific computing with Python

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Open source MPI-2 implementation

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Platform MPI 7

Description:

High performance MPI implementation (formerly HP-MPI)

Site:

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

License:

Commercial

OpenBabel

Description:

The Open Source Chemistry Toolbox

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

Site:

http://openbabel.org/

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ASE

Description:

Atomistic Simulation Environment

ASE is used to perform MD simulations within pymd.

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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Packmol

Description:

Packing Optimization for Molecular Dynamics Simulations

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

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

Site:

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

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==========

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

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Library to compute the discrete Fourier transform

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