



Scientific Computing & Modelling

References

ADF Program System

Release 2004.01

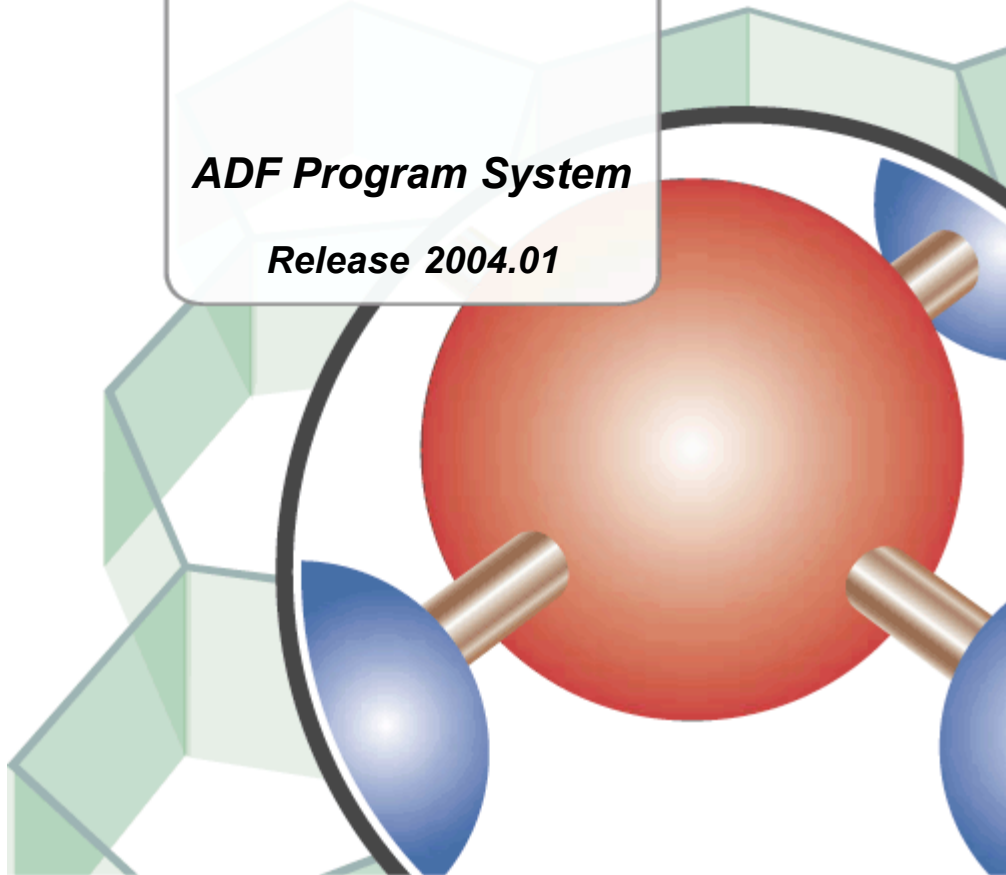


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General References

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:

For calculations with the molecular ADF code, version 2004.01:

1. G. te Velde, F.M. Bickelhaupt, S.J.A. van Gisbergen, C. Fonseca Guerra, E.J. Baerends, J.G. Snijders, T. Ziegler, 'Chemistry with ADF', *J. Comput. Chem.* **22**, 931-967 (2001)
2. C Fonseca Guerra, J G Snijders, G te Velde, and E J Baerends, *Theor. Chem. Acc.* **99**, 391 (1998)
3. ADF2004.01, SCM, Theoretical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands, <http://www.scm.com>

Optionally, you may add the following list of authors:

E.J. Baerends, J. Autschbach, A. Bérces, C. Bo, P. M. Boerrigter, L. Cavallo, D.P. Chong, L. Deng, R. M. Dickson, D. E. Ellis, L. Fan, T. H. Fischer, C. Fonseca Guerra, S. J. A. van Gisbergen, J. A. Groeneveld, O. V. Gritsenko, M. Grüning, F. E. Harris, P. van den Hoek, H. Jacobsen, G. van Kessel, F. Kootstra, E. van Lenthe, D.A. McCormack, V. P. Osinga, S. Patchkovskii, P. H. T. Philipsen, D. Post, C. C. Pye, W. Ravenek, P. Ros, P. R. T. Schipper, G. Schreckenbach, J. G. Snijders, M. Sola, M. Swart, D. Swerhone, G. te Velde, P. Vernooijs, L. Versluis, O. Visser, E. van Wezenbeek, G. Wiesenekker, S. K. Wolff, T. K. Woo, and 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.

For calculations with the periodic structures BAND code, version 2004.01:

1. G te Velde and E J Baerends, *Phys. Rev B* **44**, 7888 (1991)
2. G Wiesenekker and E J Baerends, *J. of Phys.: Condensed Matter* **3**, 6721 (1991)
3. BAND2004.01, SCM, Theoretical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands, <http://www.scm.com>

Optionally, you may add the following list of authors:

G. te Velde, E.J. Baerends, P.H.T. Philipsen, G. Wiesenekker, J.A. Groeneveld, F. Kootstra, P.L. de Boeij, J.G. Snijders

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.

In addition to these general references, references to special features are mandatory, in case you have used them. See below for details.

Feature References

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.

Frequencies, IR Intensities

(Using Numerical Differentiation of First Derivatives of the Energy)

L Fan and T Ziegler, *J. Chem. Phys.* **96**, 9005 (1992)

L Fan and T Ziegler, *J. Phys. Chem.* **96**, 6937 (1992)

Transition State search

L Versluis and T Ziegler, *J. Chem. Phys.* **322**, 88 (1988)

L Fan and T Ziegler, *J. Am. Chem. Soc.* **114**, 10890 (1992)

Analytical Second Derivatives (SD PROGRAM)

A Bércecs, R M Dickson, L Fan, H Jacobsen, D Swerhone, and T Ziegler, *Comput. Phys. Commun.* **100**, 247 (1997)

H Jacobsen, A Bércecs, D P Swerhone, and T Ziegler, *Comput. Phys. Commun.* **100**, 263 (1997)

S.K. Wolff, unpublished

IRC

L Deng and T Ziegler, *J. Chem. Phys.* **99**, 3823 (1993)

L Deng and T Ziegler, *Int. J. Quantum Chem.* **52**, 731 (1994)

ADF-BAND: Periodic Systems

Lead

See key references above, for all work with BAND

Suggested

G Wiesenekker, G te Velde, and E J Baerends, *J. Phys. C: Solid State Phys.* **21**, 4263 (1988)

G te Velde and E J Baerends, *J. Comput. Phys.* **99** (1), 84 (1992)

TDDFT IN ADF-BAND: Periodic Systems

Lead

F. Kootstra, P. L. de Boeij, and J. G. Snijders, *J. Chem. Phys.* **112**, 6517 (2000).

F. Kootstra, P. L. de Boeij, and J. G. Snijders, *Phys. Rev. B* **62**, 7071 (2000).

Suggested journal references

F. Kootstra, P. L. de Boeij, H. Aissa, and J. G. Snijders, *J. Chem. Phys.* **114**, 1860 (2001).

P. L. de Boeij, F. Kootstra, and J. G. Snijders, *Int. J. Quantum Chem.* **85**, 449 (2001).

P. L. de Boeij, F. Kootstra, J. A. Berger, R. van Leeuwen, and J. G. Snijders, *J. Chem. Phys.* **115**, 1995 (2001).

Suggested book references

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

F. Kootstra, P. L. de Boeij, R. van Leeuwen, and J. G. Snijders, in 'Reviews of modern quantum chemistry', a celebration of the contributions of Robert G. Parr, Editor K. D. Sen, World Scientific, Singapore, 2002.

Solvent Effects

C C Pye and T Ziegler, *Theor. Chem. Acc.* **101**, 396 (1999)

QM/MM

Lead

T K Woo, L Cavallo, and T Ziegler, *Theor. Chem. Acc.* **100**, 307 (1998)

Suggested

T K Woo, S Patchkovskii, and T Ziegler, *Computing in Science & Engineering*, 2000, November/December, 28-37

For AddRemove model

M. Swart, *Int. J. Quant. Chem.*, in press (2003)

Relativistic Corrections

ZORA

Lead references

E van Lenthe, E J Baerends, and J G Snijders, *J. Chem. Phys.* **99**, 4597 (1993)

E van Lenthe, E J Baerends, and J G Snijders, *J. Chem. Phys.* **101**(11), 9783 (1994)

E van Lenthe, AE Ehlers, and E J Baerends, *J. Chem. Phys.* **110**, 8943 (1999)

Suggested related references

E van Lenthe, J G Snijders, and E J Baerends, *J. Chem. Phys.* **105**(15), 6505 (1996)

E van Lenthe, R van Leeuwen, E J Baerends, and J G Snijders, *Int. J. Quantum Chem.* **57**, 281 (1996)

Pauli

Lead references

J G Snijders, E J Baerends, and P Ros, *Mol. Phys.* **38**, 1909 (1979)

P M Boerrigter, E J Baerends, J G Snijders, *Chem. Phys.* **122**, 357 (1988)

T Ziegler, V Tschinke, E J Baerends, J G Snijders, W Ravenek, *J. Phys. Chem.* **93**, 3050 (1989)

Bond Energy Analysis

T Ziegler and A Rauk, *Inorg. Chem.* **18**, 1558 (1979)

T Ziegler and A Rauk, *Inorg. Chem.* **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

Time-Dependent DFT: Response Properties

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, *Comput. Phys. Commun.* **118**, 119, (1999)

Excitation Energies and Oscillator Strengths

Lead reference

S J A van Gisbergen, J G Snijders, and E J Baerends, *Comput. Phys. Commun.* **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, *J. Am. Chem. Soc.* **121**, 10356 (1999)

Polarizabilities

Lead

S J A van Gisbergen, J G Snijders, and E J Baerends, *J. Chem. Phys.* **103**, 9347 (1995)

Suggested

V P Osinga, S J A van Gisbergen, J G Snijders, and E J Baerends, *J. Chem. Phys.* **106**, 5091 (1997)

Hyperpolarizabilities

Lead

S J A van Gisbergen, J G Snijders, and E J Baerends, J. Chem. Phys. **109**, 10644 (1998)

Suggested:

S J A van Gisbergen, J G Snijders, and E J Baerends, Phys. Rev. Lett. **78**, 3097 (1997)

Dispersion Coefficients

Lead

V P Osinga, S J A van Gisbergen, J G Snijders, and E J Baerends, J. Chem. Phys. **106**, 5091 (1997)

Suggested

S J A van Gisbergen, J G Snijders, and E J Baerends, J. Chem. Phys. **103**, 9347 (1995)

Raman Scattering

S J A van Gisbergen, J G Snijders, and E J Baerends, Chem. Phys. Lett. **259**, 599 (1996)

Circular Dichroism (CD)

Lead

J. Autschbach, T. Ziegler, J. Chem. Phys. **116**, 891 (2002)

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

Lead

J. Autschbach, T. Ziegler, J. Chem. Phys. **116**, 891 (2002)

J. Autschbach, S. Patchkovskii, T. Ziegler, S.J.A. van Gisbergen, and E.J. Baerends, J. Chem. Phys. **117**, 581 (2002)

ESR/EPR parameters

G-tensor: Zeeman interaction

Lead references (EPR/NMR program)

G. Schreckenbach and T. Ziegler, J. Phys. Chem. A 1997, **101**, 3388 (for ESR/EPR g-tensor)

S. Patchkovskii and T. Ziegler, J. Phys. Chem. A 2001, **105**, 5490 (for high-spin ESR/EPR g-tensor)

Lead reference (ADF)

E. van Lenthe, A. van der Avoird, and P.E.S. Wormer, *J Chem Phys* **107**, 2488 (1997)

A-tensor: Nuclear magnetic dipole hyperfine interaction

Lead reference

E. van Lenthe, A. van der Avoird, and P.E.S. Wormer, *J Chem Phys* **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, *J. Chem. Phys* **112**, 8279-8292 (2000)

NMR Chemical Shifts

Lead reference

G Schreckenbach and T Ziegler, *J. Phys. Chem.* **99**, 606 (1995)

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G Schreckenbach and T Ziegler, *Int. J. Quantum Chem.* **60**, 753 (1996)

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S K Wolff and T Ziegler, *J. Chem. Phys.* **109**, 895 (1998)

S K Wolff, T Ziegler, E van Lenthe, and E J Baerends, *J. Chem. Phys.* **110**, 7689 (1999)

NMR spin-spin coupling

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J. Autschbach and T. Ziegler, *J. Chem. Phys.* **113**, 936 (2000)

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R M Dickson and T Ziegler, *J. Phys. Chem.* **100**(13), 5286 (1996)

J Khandogin and T Ziegler, *Spectrochimica Acta* **55**, 607 (1999)

J. Autschbach, T. Ziegler, *J. Am. Chem. Soc.* **123**, 3341 (2001)

J. Autschbach, T. Ziegler, *J. Am. Chem. Soc.* **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*.