

References

ADF Program System
Release 2002.01

SCIENTIFIC COMPUTING & MODELLING NV
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27 February, 2002

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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 2002.01:

- 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 ADF2002.01, 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.A. Autschbach, A. Bércecs, 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, 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 2002.01:

- 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 BAND2002.01, SCM, Theoretical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands, <http://www.scm.com>

Optionally, you may add the following list of authors:

G. te Velde, G. Wiesenekker, P.H.T. Philipsen, J.A. Groeneveld, E.J. Baerends

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

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TRANSITION STATE SEARCH

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ADF-BAND: PERIODIC SYSTEMS

Lead

See key references above, for all work with BAND

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Suggested related references

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

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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)

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G-tensor: Zeeman interaction

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A-tensor: Nuclear magnetic dipole hyperfine interaction

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EPR/NMR PROGRAM

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

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

