References

ADF Program System
Release 2002.03

SCIENTIFIC COMPUTING & MODELLING NV
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December 11, 2002

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 2002.03:

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 ADF2002.03, 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. 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, 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 2002.03:

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. BAND2002.03, 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

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ADF-BAND: PERIODIC SYSTEMS

Lead

See key references above, for all work with BAND

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

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