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COMPUTER SOFTWARE
REVIEWS

Amsterdam Density Functional 2005. Scientific Computing and Modelling NV, Vrije Universiteit, Theoretical Chemistry, De Boelelaan 1083, 1081 HV Amsterdam, the Netherlands. http://www.scm.com. See Web site for pricing information.

Amsterdam Density Functional (ADF) is an electronic structure package primarily developed by chemistry groups in Amsterdam under Prof. Baerends, in Calgary under Ziegler, and in Groningen under Snijders, as well as by several other research groups. A great overview of the functionality of this program is given in the literature: te Velde, G.; Bickelhaupt, F. M.; Baerends, E. J.; Fonseca Guerra, C.; van Gisbergen, S. J. A.; Snijders, J. G.; Ziegler, T. Chemistry with ADF. *J. Comput. Chem.* **2001**, *22*, 931−967 and Fonseca Guerra, C.; Visser, O.; Snijders, J. G.; te Velde, G.; Baerends, E. J. Parallelisation of the Amsterdam Density Functional Program. In *Methods and Techniques for Computational Chemistry*; Clementi, E., Corongiu, C., Eds.; STEF: Cagliari, 1995; pp 303−395.

This program package is available for Linux, Windows, Mac OS X, and several Unix platforms. ADF requires no more than 256 MB of memory, but at least 512MB or 1GB are suggested for large calculations. The software was easy to set up on the two platforms used in the review, Linux RedHat 9 and Windows XP. The user can either download the precompiled executables for the compatible platforms mentioned or download the source code directly if necessary. The documentation is extensive and well organized into several sections, including installation, tutorial, and detailed instructions about the program package. Examples are also given in the documentation, and the input/output can be found in the directory where the program has been installed. The Web site is very useful in providing links to more documentation and possible help, as well as a list of related journal articles.

This package allows calculation of ground- and excited-state energies, as well as harmonic vibrational frequencies, optimized structures, and even molecular properties such as NMR spin coupling or NMR spin−spin coupling. It can also treat problems of solvation and conduct transition state searches. The methods used are primarily DFT, although it also allows the user to use QM/MM methods in order to treat larger systems. The Sybil and Amber force fields are provided with ADF and can easily be modified by the user. One can choose between several exchange and correlation functionals that can be parametrized including Becke-Perdew, Becke exchange with LYP correlation, Perdew-Wang 1991, and several others. The choice of basis sets included in ADF is limited, but it is possible to create new sets if needed. Analytical second derivatives are available in this program package, but their efficiency is still limited and so far only work for a few functionals. Another module in ADF called Band allows the user to study bulk crystals and polymers. It is a useful tool for studying the phenomena of chemisorption or reactions on surfaces. A valuable feature is the possibility to perform parallel calculations on large clusters of computers. Two types of parallel architecture are supported: message passing interface and parallel virtual machine.

One can either use the graphical interface to create the ADF input file by choosing between several groups of molecules (amino acids, DNA, cyclic hydrocarbons, etc.) and including additional atoms to obtain the desired structure or create one's own input file from scratch as is done with most electronic structure packages. For larger calculations, ADF input files can be created from a Protein Data Bank file by using a contributing software, pdb2adf, that is available on the SCM website, making it easier to run calculations with ADF on larger and biologically relevant molecules. The graphical interface includes several subprograms and viewing tools. The molecular orbital density surfaces are well rendered and are easily customizable. The user can visualize molecular energy levels to get a better grasp of the system but also look at the different vibrational modes or the different steps of a procedure for optimization or for searching for a transition state. One can also perform simulations of IR, Raman, and electronic spectra as well as visualize the density of states. This feature makes the program package attractive for experimental and computational groups in search of quick, easy, but approximate simulations of molecular spectra.

We recommend ADF for its ease of use and treatment of various chemical problems that are important to academia and industry, although one should keep in mind that ADF is limited to calculations using DFT and molecular force field methods. It cannot perform any calculations using MP2, CI, or CC methods. However ADF provides great flexibility and can be used for a wide range of chemical applications from inorganic chemistry to biology and surface science.

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