

Enhancing QTAIM Implementation in ADF Software

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The Quantum Theory of Atoms in Molecules (QTAIM)¹ facilitates the analysis of electron density within molecular systems, offering insights into atomic interactions and structural features such as chemical bonds, rings, and cages.

Previously, the application of QTAIM within the Software for Chemistry & Materials (SCM) suite was limited. Our work specifically addresses this in the Amsterdam Density Functional (ADF)², where we have expanded the characterization of structural motifs, including atoms involved in rings and cages. Additionally, we have refined the decomposition of the dipole moment into its intra- and interatomic components³. Moreover, we developed a script using the Python Library for Automating Molecular Simulations (PLAMS)⁴ to compute atomic polarizabilities. Together, these developments not only enhance the functionality of the ADF software within the SCM suite but also broaden the scope of QTAIM applications, paving the way for research opportunities in chemistry and materials science.

Consequently, our implementation is poised to facilitate several applications such as UV-visible absorption and emission spectra, or electronic circular dichroism under realistic biological conditions, through the Polarizable Embedding (PE) approach⁵. Furthermore, our code can be extended, for example, to crystallography applications through integration with the BAND software (also part of the SCM suite).

Keywords: ADF, SCM, QTAIM, Polarizability

¹R. F. W. Bader, *Atoms in Molecules: A Quantum Theory* (1994).

²G. te Velde, F. M. Bickelhaupt, E. J. Baerends, C. Fonseca Guerra, S. J. A. van Gisbergen, J. G. Snijders, and T. Ziegler. *J. Comput. Chem.* 22(9) (2001) 931-967.

³T. A. Keith. *The Quantum Theory of Atoms in Molecules Atomic Response Properties* (2007)

⁴M. Handzlik, B. van Beek, P. Melix, R. Rüger, T. Trnka, L. Ridder, and F. Zapata, *PLAMS, Python Library for Automating Molecular Simulations*.

⁵M. T. P. Beerepoot, A. H. Steindal, N. H. List, J. Kongsted, and J. M. H. Olsen. *Journal of Chemical Theory and Computation* 12(4) (2016) 1684–1695