ChemOffice Reviews

Molecular Modeling with the ChemOffice Ultra 4.5 Program Suite

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Marc Baaden is a chemical engineer at the European Higher Institute of Chemistry of Strasbourg. He is currently preparing a PhD thesis in the field of molecular dynamics investigating synergistic effects in liquid-liquid extraction of ions.

The first impression

After installing the ChemOffice Ultra 4.5 pack on my computer (a Pentium 150 with 48 MB RAM), I started to explore the user's guides (one for each program), and was pleased to discover a sound documentation of the software suite. The manuals were easy to read, comprehensive and provided a complete summary of the program features as well as some hints for the more advanced user. The next step was an "on-the-job training" using the many examples given in the software documentation.

What about Molecular Modeling?

After these first steps I was keen on learning more about the Chem3D program, which seemed to be the ChemOffice module that was most related to my work as a theoretical chemist. Chem3D proved as a useful tool for examining and visualizing three dimensional molecular models, most often issued from Molecular Dynamics ("MD") calculations carried out with the AMBER[1] software or from ab initio studies performed with GAUSSIAN 94.[2] The computational jobs were done on supercomputers or workstations since the model systems exceeded my computer's capabilities.

A major requirement for using Chem3D in my daily work was the possibility to transfer results from AMBER and GAUSSIAN jobs to Chem3D.

It works!

The PDB file format proved to be suitable for visualizing instantaneous microscopic views observed during MD runs. A very helpful Chem3D feature was to read in connectivity information provided in the AMBER PDB file, in order to preserve the model system as it was simulated by MD. Furthermore creating "new elements" enabled Chem3D to recognise the specific atom types of solvent molecules as they are treated by AMBER and to define their visual aspects. By this procedure it was possible to import PDB files obtained from snapshots of the MD runs into Chem3D, then prepare a suitable view of the model system and copy the final figure to any other windows application. Figure 1 below shows one of the model systems we are currently investigating at Professor G. Wipff's MSM laboratory in Strasbourg, France[3] -- a Calix[4]arene complex at a water/chloroform interface.

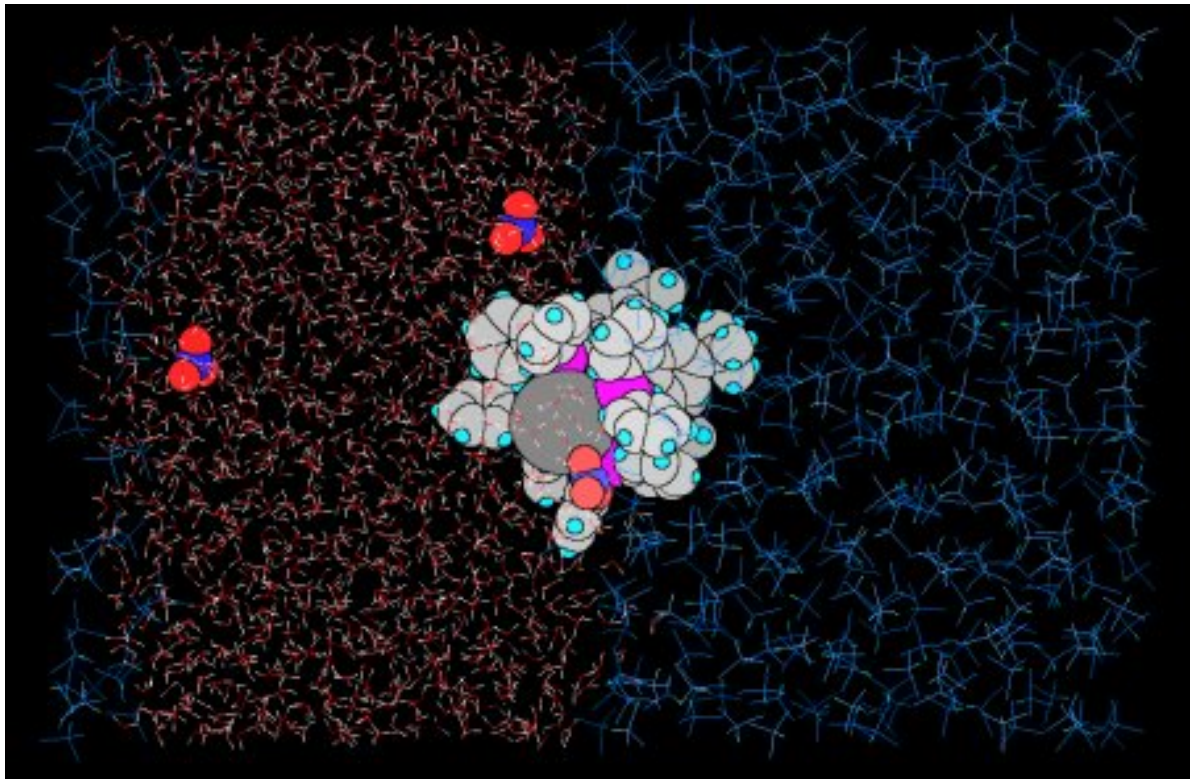

Figure 1. A calix[4]arene complex at the water/chloroform interface, shown with 3 nitrate counter ions.

On the way to first principles

The visualization of GAUSSIAN results obtained on other computer platforms was very easy. Once a formatted checkpoint file (GAUSSIAN utility formchk) and a cube file (GAUSSIAN utility cubegen) were obtained, Chem3D could interpret them without any difficulty. The Chem3D module can visualize optimized geometries, molecular orbitals and several kinds of molecular surfaces obtained by first principles calculations. An example is given in figure 2 which shows the total spin density as well as alpha and beta spin densities of the 2-cyano-2-propyl radical. The surface was obtained from an unrestricted Hartree Fock calculation performed with GAUSSIAN 94 using the 6-31G basis set.

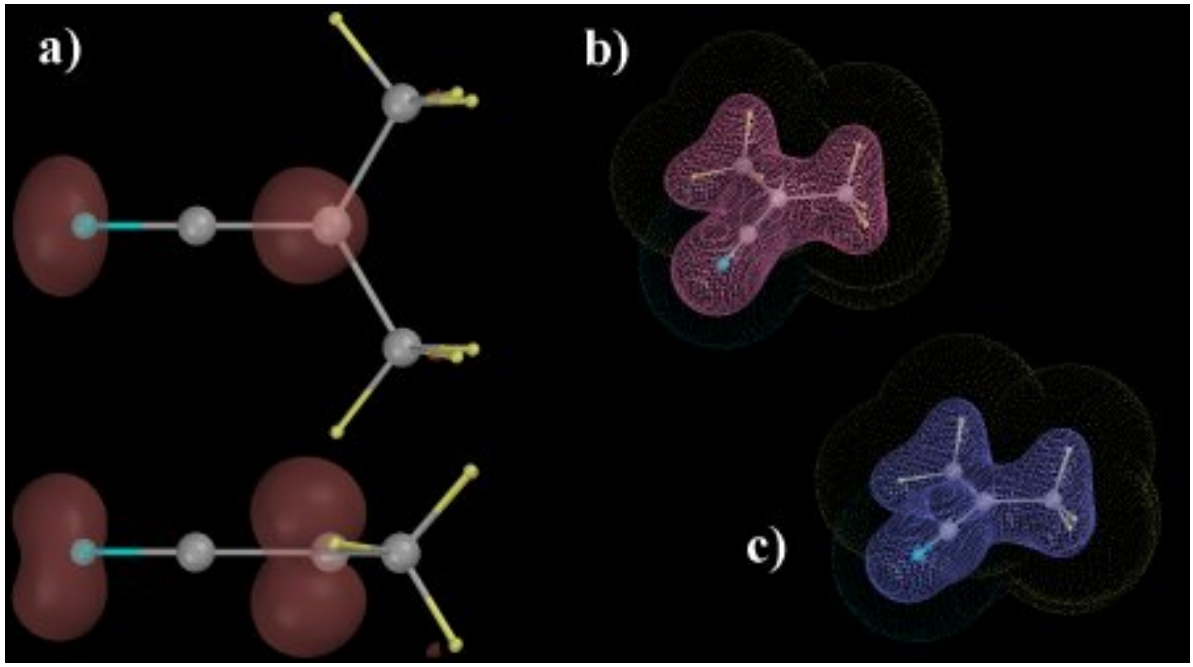

Figure 2. Molecular surfaces depicting the "radical-ness" of the 2-cyano-2-propyl radical. Results were obtained with GAUSSIAN 94 at UHF/6-31G level of theory. a) total spin density surface, b) alpha spin and c) beta spin density surface, both surrounded by the molecule's solvent accessible surface for water (1.4 Å). All surfaces were calculated on a 90x88x65 grid with an isovalue of 0.02 a.u.

Chem3D also contains several computational modules that allow to conduct semi-empirical calculations, MM2 Molecular Mechanics and Dynamics runs and to predict molecular properties. I also appreciated the possibility to compute molecular orbitals by the extended Huckel method. It is a very convenient and fast procedure to display molecular orbitals. Figure 3 shows the HOMO of tetraphenylporphyrin calculated by this method and visualized with Chem3D.

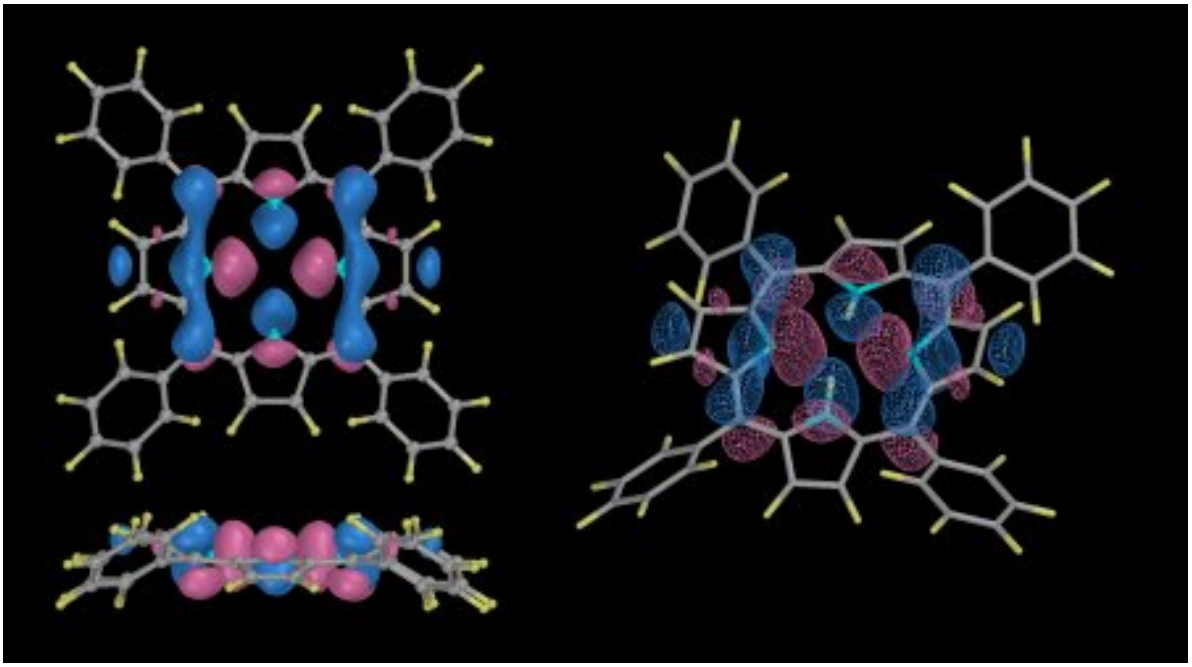

Figure 3. The HOMO of tetraphenylporphyrin seen from different angles (mapped on a 100x100x100 grid with an isovalue of 0.01 a.u.).

Everyday tasks made easy

My principle use of ChemOffice was the preparation of high quality figures suitable for publication or report preparation. In this context it should be pointed out, that it is possible to transform Chem3D models into 2 dimensional figures with ChemDraw and vice versa.

The options provided with ChemDraw to modify 2D structures are very powerful and turn the preparation of comprehensive structure charts into an easy job.

No problems?

There were some problems, bugs and flaws as in any software package. The major ones for me were the lack of the GAUSSIAN interface to handle Z-matrices, which is essential for building molecular structures of a given symmetry group. Generally speaking, I would not recommend the GAUSSIAN interface for the preparation of job input files, at least if your intention is to perform sophisticated ab initio calculations such as BSSE, use of pseudo-potentials and the like, but in turn I can highly recommend Chem3D for the visualization of the results. There is, however, one feature I would like to be included in the visualization module: hidden surfaces. Printed versions of figures depicting molecular surfaces are often difficult to read because they are too complex. Including simple surface representation modes like the existing wire mesh combined with hidden surfaces would turn the figures more comprehensive.

Another general problem is that the programs are quite demanding in CPU power and available memory. I managed to "crash" the Chem3D module several times.

Summary

My overall impression on this ChemOffice Ultra release is very positive. Although I experienced some trouble from time to time, I think that these programs are a good choice if you are interested in an integrated package useful for building, analyzing, visualizing and drawing structures. The software has become an useful companion for my daily work in the field of Molecular Modeling.

Furthermore I would like to point out that the technical support provided to registered users is excellent. The support staff helped me more than once and their responses were very useful.

For further or more detailed questions, I invite you to have a look at my website at http://crypt.u-strasbg.fr/marc where you can find some examples as well as my contact information.

References

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(2) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Gill, P. M. W.; Johnson, B. G.; Robb, M. A.; Cheeseman, J. R.; Keith, T. A.; Petersson, G. A.; Montgomery, J. A.; Raghavachari, K.; Al-Laham, M. A.; Zakrzewski, V. G.; Ortiz, J. V.; Foresman, J. B.; Peng, C. Y.; Ayala, P. A.; Wong, M. W.; Andres, J. L.; Replogle, E. S.; Gomperts, R.; Martin, R. L.; Fox, D. J.; Binkley, J. S.; Defrees, D. J.; Baker, J.; Stewart, J. P.; Head-Gordon, M.; Gonzalez, C.; Pople, J. A. Gaussian 94 (Revision D.2); Gaussian, Inc.: Pittsburgh PA, 1995.
(3) Wipff, G. et al.; J. Phys. Chem. B 1998, 102, 245-256.

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