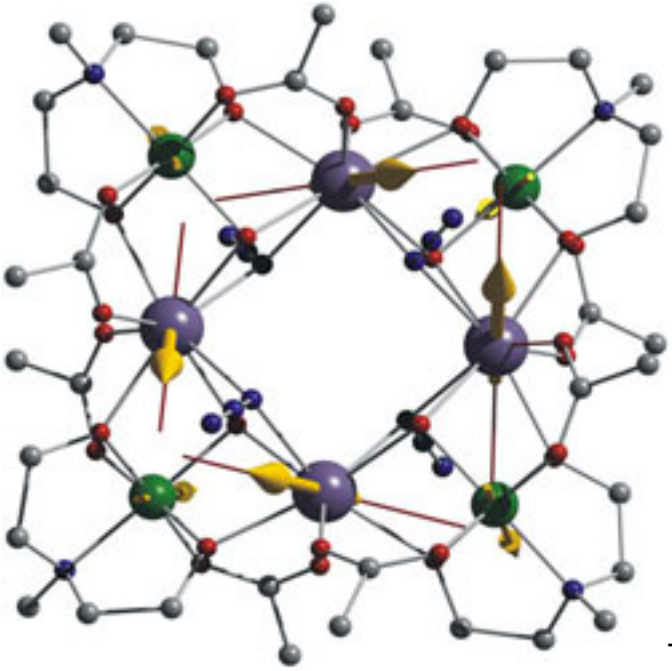
Spin paper closes knowledge gap on density functional theory



The review paper on the consideration of spin in density functional theory (DFT), published by the scientists Dr. Christoph Jacob from the Center for Functional Nanostructures (CFN) of Karlsruhe Institute of Technology and Professor Markus Reiher from ETH Zurich, functions to close a major knowledge gap in theoretical chemistry.

Density functional theory (DFT) is an important tool within the field of theoretical chemistry. It is used to calculate the properties of molecules and solids, such as binding lengths and energies.

For the time being, molecules with paired electrons only can be calculated using DFT. For molecules with unpaired electrons, also called open-shell systems, DFT cannot yet be applied in a satisfactory manner. Unpaired electrons lead to a magnetic moment, the spin, and its consideration by DFT remains quite challenging.

In transition metals and their compounds, these unpaired electrons offer a rich and complex chemistry, making them interesting for a number of applications. Change of spin in bio-inorganic reactions, for instance, may be responsible for a transition metal complex acting as a catalyst. Transition metal clusters in single molecule magnets are integral as connections of storage elements in (quantum) information processing.

The large scope of applications explains the high scientific interest in calculating the behavior of open-shell systems using theoretical methods. In past years, scientists Jacob and Reiher began systematic studies in this field and developed solution approaches. Currently, they have published their detailed results in the

International *Journal of Quantum Chemistry* in the form of a tutorial that is highly useful for both beginners and advanced practitioners.

“Understanding of the underlying exact theory is a prerequisite for the development of a reliable approximation method. That is why we first sum up these fundamentals,” Jacob says.

The authors explain the non-relativistic treatment of spin for a single electron – the subject of many basic studies in quantum mechanics. They then analyze the treatment of spin using the Hohenberg-Kohn and Kohn-Sham DFT. Various methods of considering spin in DFT are described and analyzed. Jacob and Reiher also study the relativistic DFT. Finally, proposals are made as to how spin approximation can be improved within the DFT.

Density functional theory (DFT)
In the 1960s, fostered by the newly emerging computer generation, quantum chemistry developed into its own field of theoretical chemistry. Until then, it had been scarcely possible to describe complex structures, such as molecules, using mathematical equations to calculate their behavior. Although the underlying laws were well known, they were too complex to be managed using calculations alone. The calculation of chemical bonds between the atoms of a molecule became possible only after the development of approximation methods and the more ubiquitous use of computers in the 1960s. In chemistry, this development marked the transition from an experimental to a computable science. Two leading fundamental scientists of that time were Walter Kohn and John A. Pople. In 1998, they were awarded the Noble Prize for Chemistry, Kohn for the development of the DFT and Pople for the development of computation methods in quantum chemistry. Since then, computing capacity has multiplied exponentially and DFT has developed further, such that it can now be used for larger and more specific structures.

Closing the Gap in Spin Calculations for Open Shell Systems [1]

Source: Karlsruhe Institute of Technology [2]

Links:
[1] http://www.chemistryviews.org/details/ezine/2525611/Closing_the_Gap_in_Spin_Calculations_for_Open_Shell_Systems.html
[2] http://www.kit.edu/english/