



Molecular Electronics on the North West Grid

Work on NW-GRID is partly aimed at developing a state-of-the-art suite of simulation tools, capable of predicting material-specific properties of hybrid nano-structures. This project will produce a major leap forward, by forming a bridge between *ab initio* electronic structure calculations, nano-scale transport and molecular electronics. Devices and materials relevant to current and future industrial needs will be modeled and results will be used to initiate pre-competitive industry-based research projects.

This new capability will lead to a database of tight binding parameters for materials and their interfaces, which can be used to predict and optimise the properties of nano-structures of arbitrary complexity, e.g. Figure 1.

In parallel with this over-arching activity, a number of new projects are being tackled, examples of which include:

- Developing a theory of superconducting and ferromagnetic proximity effects in carbon nano-tubes and hybrid metallic nano-structures.
- Developing a theory of how the proximity to step edges on a semiconductor surface can be used to organize nano-tubes.
- Understanding the effects of docking molecules on transport through nano-tubes.
- Modeling transport through single molecules of immediate interest to experimental programmes in QinetiQ and elsewhere, including

conductance through mono-molecular arrays.

- Investigating quantum properties of polyacene crystals, which are currently the subject of intense worldwide investigation.

In a first series of runs, the DFT code SMEAGOL (Spin and Molecular Electronics in an Atomically Generated Orbital Landscape) has been used to calculate the conductance through twisted single molecule junctions based upon bi- or tri-phenyl rings with amine link groups, see Figure 2. The calculations to find the lowest energy configurations of various molecules takes some time to complete and the unique opportunity to use the full computing power of the NW-GRID to complete this initial stage was fortuitous as it could give us the edge (in terms of time) over most other research groups in the field. After initial tests to confirm that we had standardised results across the Grid, we proceeded with the calculations, which were successful and now form a core of data which has been used to complete a research publication [1].

This work was carried out by Colin Lambert, Iain Grace, Victor Garcia-Suarez, Skon Sirichantaropass and Chris Finch from University of Lancaster.

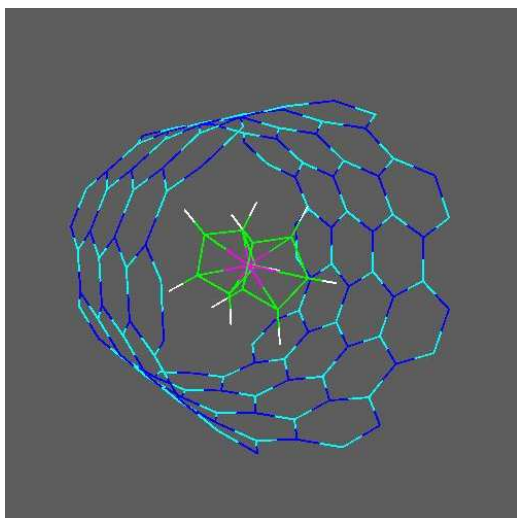


Figure 1: The atomic positions of Cobaltocene inside an "armchair" carbon nano-tube.

Four researchers were principally involved in the job submissions, and they ran a variety of jobs of different sizes. We had set up a NW-GRID client gateway server with the necessary Globus components to run gsi and apart from the time taken to transfer files from this machine to the working site, all the users found the Grid accessible and efficient. Naturally once the initial files are transferred the process is relatively easy. This is improved even more by using a client toolkit such as GROWL. The main advantage as far as the NW-GRID is concerned has to be that we have a core of users who are familiar with job submissions and from this critical number it is likely that all the group will use the Grid in the future.

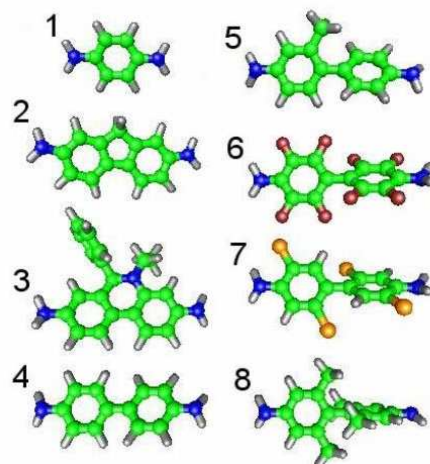


Figure 2: Possible constituents of molecular wires reveal a dependency of conductance on angle of rotation.

SMEAGOL is jointly developed by Universities of Lancaster and Oviedo (Spain) and Trinity College Dublin (Ireland). Further information about SMEAGOL and its academic license can be found at <http://www.smeagol.tcd.ie>.

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For more information about this work please contact Dr. Steven Bailey at University of Lancaster.

[1] C.M. Finch, S. Sirichantaropass, S.W. Bailey, I.M. Grace, M. Garcia-Suarez and C.J. Lambert *Conformation Dependence of Molecular Conductance: Chemistry versus Geometry* (March 16th, 2007)