Final Report: Interdisciplinary Approaches to Functional Electronic and Biological Materials

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- Purpose of the visit

To investigate the induced magnetic effect of metallorganic molecules on magnetic substrates with and without graphene. The questions to be investigated included 1) the local stucture of the magnetic substrates, namely Co and Ni, 2) the local structural changes of the metallo-porphyrin on adsorption on to the pure substrate and one layered with graphene, 3) the physiosorption and chemisorption cases would be investigated and the energy barriers quantified, 4) the effects of graphene on the induced magnetic properties of the metal centre of porphyrin molecules.

The aim of the short visit is to try and answer some the questions highlighted above. The Materials Theory Division at the Dept. of Physics and Astronomy, headed by Prof. Olle Eriksson, has a lot proven track record in the implementation of density functional theory methods and therefore would be an ideal place to establish links. The visit will also include a departmental presentation and a poster presentation at the "Functional Metalorganics — Magnetism, structure, transport FM2011" conference to be held between 30 May – 01 June 2011.

Due to Visa issues this trip was divided into two parts totalling

- Description of the work carried out during the visit

DFT theory calculations were set up on local and national super computers within Sweden. Access accounts needed to be set up which took a few days. Discussions with Barbara Brena working on the project but with a Co substrate and Sumanta Bhandary working on the Ni (111) substrate were undertaken. I was contributing with calculations on Ni (100) substrate. In all cases a systematic study of porphyrin position and distance from the surface were carefully set up. A discussion of adding dispersive forces which are not implicitly included in DFT was concluded with agreement that at least the Grimme method within the VASP code should be used.

- Description of the main results obtained

The main results are summarised:

1) The magnetic moments on the metal centre are sensitive to the position (bridge, hollow or top) relative to the substrate atoms.
2) Very interesting correlations between the different Ni orientations were found and will be published soon. This is the first extensive study where the effect of different orientated surfaces has been investigated.
3) We are still investigating the effect of grapheme and hoping to collaborate with an experimental group in Duisburg-Essen to understand better the results.
4) Physiosorption and chemisorption is very much dependent on the site of the porphyrin on the substrate and the high spin is always only found in the case of physiosorption.
5) The ligands also play a vital role in determining the lowest energy configuration.

- Future collaboration with host institution *(if applicable)*

Future collaborations are underway with a STINT grant (Swedish institute for international collaboration) between Barbara Brena and myself (Pooja M. Panchmatia).

- Projected publications/articles resulting or to result from your grant

Two publications have been projected and are awaiting final calculations to be completed by both parties.

- Other comments *(if any)*

As mentioned earlier due to Visa issues this trip was divided into two trips in the end although the travel expense did not exceed 500 euros.
The first trip was from 28th June 2011 – 03rd July 2011 (6 days)
The second trip was from 30th August 2011 – 03 September 2011 (5 days)