Research Networking Programmes

Science Meeting – Scientific Report

"Theory of metal atoms, clusters and nanoparticles interacting with organic matter"

Application Reference N° 5761

1) Summary

Due to recent progress in nano-fabrication there is a large, growing interest in stabilized metal-organic hybrids. However, at present not many computational ab-initio studies have been performed and they are scattered across different fields and communities. The workshop goal was then to address current challenges and successful methods to study the electronic properties of organo-metal nanocomposites bringing together leading scientists working both on ground and excited state electronic properties of organic stabilized metal complexes.

The total number of participants was slightly increased to 32 out of the 30 initially planed. There were 17 invited speakers and 3 contributed speakers. Out of the invited speakers, a percentage of 41 % were women, comparable to the ratio typically reached in the best conference in clusters, the Gordon Research Conference on Noble Metal Nanoparticles (with for example 32% women speakers in 2012). The format of talks with 10 minutes reserved for discussions prove to be adequate for the mixture of communities that was present. All the sessions were fully attended as can be seen from

the picture taken in the final talk. Feedback from the participants was very high. It was expressed personally to the organizers that such a space for discussing advances in different communities is extremely needed. It is expected this workshop will increase the number of computational scientists doing research in these systems, strengthen the theoretical community and therefore will boost the scientific developments in this very complex research direction.

2) Description of the scientific content of and discussions at the event

Talks and generated discussions

How to compute accurately metal-organic electronic properties?
One the central topics of the workshop was how to treat the electronic gap and energy levels for charge transfer accurately from simulations. In this topic Noa Marom showed that for TiO protected clusters the GW approach was the best closely followed by DFT with hybrid functionals (PBE0). The inclusion of long-range corrected or hybrid functionals also was included in the talks of Vlasta Bonacic-Koutecky, Roy Johnston and Stephan Kummel. This sample of accurate electronic-structure reasearch shows that it is becoming a standard practise to not rely on the pure GGA functionals. The main problem with hybrid functionals is the need of an extra parameter. During his talk, S. Kummel showed his most recent local hybrid functional that address the problem. It was asked by Miguel Caro how it would compare to normal hybrid and S. Kummel answered it has the same computational cost. Other effects that were discussed include two-photon adsorption (V. Bonacic-Koutecky), nuclear quantum effects (M. Rossi), van der Waals dispersion (A. Tkatchenko) and strong relativistic effects (E. Pahl). For every one of these aspects the speakers showed state-of-the-art methods that successfully are treating them and will hopefully be included in standard calculations in the future.

How to reach simulations of larger metal-organic systems in the quantum level?
A talk from Arash Mostofi showed impressive results in linear scaling DFT as a promising methodology. There was a question from Maria Loi on the crossover between cubic scaling and linear scaling for a given system and A. Mostofi answered it is an issue that depends on the system itself. A. Mostofi explained it is not given in advance if there will be a gain but when it works is a reliable method. Another talk from Miguel Caro showed recent work on orbital-free DFT where the main problem is the transferability of kinetic functionals away from atoms. Stephan Kummel noted the extreme difficulty of the problem and it was discussed which strategy for developing kinetic functionals are available. Caro noted that there is no currently testing of the most promising state-of-the-art functionals (like those coming from machine learning) but that it is something that it is hoped to be performed in the future.

How to perform structural search computationally and efficiently?
Jaakko Akkola explained that traditionally in the thiolated protected community it has been mainly used the educated-guess approach to propose structures. Many of the talks focused on answering the same question computationally for different type of systems. Marom showed genetic algorithms specifically adapted to TiO protected clusters. Roy Jhonston showed genetic algorithms for mixed gold-silver clusters and announced the algorithm is being added to the open-source ASE interface. Silvana Botti also discussed

GA for bulk materials while M Beltran showed a configurational search on mixed Ru-gold clusters guided by IR experiments.

State-of-the-art experiments

The workshop had several leading experimentalists that participated and greatly enhanced the discussions. T. Tsukuda opened the workshop showing his advancements characterizing new polymer-stabilized and thiol-protected gold clusters where the structure is still unknown. Several talks focused on DNA-stablized silver cluster systems (J. Muller, A. Lopez-Quintela, S. Swaswey) where interesting applications in sensing and imaging have been proved.

Tutorials

In the workshop organized two years ago the organizers relied on the use of tutorials to help the communication between communities but in this workshop the tutorials were not included. It is a conclusion from the organizers that in a follow-up workshop such tutorials should be organized again.

3) Assessment of the results and impact of the event on the future directions of the field

In the workshop all the sessions were attended by the majority of all participants showing the interest the talks created. In the discussions, both theoretical and experimental researchers participated actively making the related objective fulfilled. The impact on the computational modelling of quantum properties of interacting organo-metal nanocomposites is expected to be important. Several research groups will include projects in this direction and a strengthen of the theoretical community has been created. A follow-up workshop in two years would support the development of this community in this very challenging research direction.

4) Annexes 4a) and 4b): Programme of the meeting and full list of speakers and participants

SNM15 Program

Theory of metal atoms, clusters and nanoparticles stabilized by organic matter workshop

June 10-12 2015 Helsinki, Finland

Wednesday 10.6

08:30 Registration

Chair O. Lopez-Acevedo

09:00 Prof. Tatsuya Tsukuda, Tokyo University (Japan), Toward precise control of morphology and interfacial structure of ligand-protected gold clusters [pdf]

09:45 Prof. Vlasta Bonacic-Koutecky, Humboldt-Universität zu Berlin (Germany), Tuning optical and catalytic properties of ligated silver clusters by synergistic role of metallic and organic subunits [pdf]

10:30 COFFEE

10:50 Prof. Silvana Botti, Friedrich-Schiller Universität Jena (Germany), Electronic excitations in Cu-chalcogenide and perovskite solar cell absorbers [pdf]

11:35 Prof. Maria Antonietta Loi, University of Groningen (Netherlands), Colloidal Quantum Dot Solids: determination of the energy levels and tuning of the electronic properties [pdf]

12:20 LUNCH

Chair P. Rinke

15:00 Prof. Arash Mostofi, Imperial College London (UK), Challenges and opportunities in large-scale electronic structure simulations [pdf]

15:45 Prof. Jaakko Akola, Tampere University (Finland), Small Au nanoparticles quantum confinement effects and atomic scale simulations of interactions in biological environments [pdf]

16:30 COFFEE

16:50 Dr. Miguel A. Caro, Aalto University (Finland), Orbital-free density functional theory: looking back to the roots of DFT [pdf]

17:10 Dr. Mariana Rossi, University of Oxford (UK), Dynamics of polypeptides from first principles for electrons and nuclei (and towards metal-peptide interactions) [pdf]

17:55 END

Thursday 11.6

Chair TBA

09:00 Prof. Jens Müller, University of Münster (Germany), DNA duplexes with silver(I)-mediated base pairs [pdf]

09:45 Prof. Stephan Kümmel, Bayreuth University (Germany), Metal nano alloys – insights from DFT and insights into DFT [pdf]

10:30 COFFEE

10:50 Dr. Elke Pahl, Massey University Auckland (New Zealand) , Mercury Clusters and the Solid: Challenges of an Ab Inito Description [pdf]

11:35 Prof. Noa Marom, Tulane University (US), Toward Computational Design of Cluster-Based Functional Nano-Structures [pdf]

12:20 LUNCH

Chair S. Kummel

14:00 Steven Swaswey, University of California Santa Barbara (US), Clusters with a twist: fluorescent silver clusters stabilized by DNA [pdf] and Prof. Elisabeth Gwinn, University of California Santa Barbara (US), DNA templates silver clusters with magic sizes and colors for multi-cluster fluorescent assemblies [pdf]

14:45 Prof. Roy Johnston, University of Birmingham (UK), Combining Theory and Experiment to Determine the Structures of Sub-nanometre Metal Clusters [pdf]

15:30 COFFEE

15:50 Dr. Olga Syzgantseva, Aalto University (Finland), Excited state charge transfer in the hybrid perylene - titanium oxide system: an ab initio study [pdf]

16:10 Prof. M. Arturo López Quintela, University of Santiago de Compostela (Spain), Small metal clusters without protecting ligands: synthesis, catalytic properties and DNA interaction [pdf]

16:55 END

18:00 DINNER

Friday 12.6

Chair E. Pahl

09:00 Dr. Ilari Filpponen, Aalto University (Finland), Luminescent biohybrid nanomaterials from nanocellulose and carbon dots (CDs) [pdf]

09:45 Prof. Marcela Beltrán, Universidad Nacional Autónoma de México (Mexico), Probing Oxygen intake by Au_nRh_m (n=1-7, m=1-2) Clusters : A Density Functional Theory and Anion Photoelectron Study [pdf]

10:30 COFFEE

10:45 Jukka Hassinen, Aalto University (Finland), SIMPLE AND EFFICIENT SEPARATION OF ATOMICALLY PRECISE NOBLE METAL CLUSTERS [pdf]

11:15 Dr. Alexandre Tkatchenko, Fritz Haber Institute of the Max Planck Society (Germany), Collective Dispersion Energy Effects in the Accurate Description of Structure and Stability of Molecules on Surfaces [pdf]

12:00 Concluding remarks

12:15 LUNCH

Important note on location:

The workshop is going to be held in the Main Building Otakaari 1, first floor.

Wednesday morning the workshop room is **Y122 D**. For the rest of the workshop (Wednesday afternoon, Thursday and Friday) the room is **A123 A1**.

List of speakers

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Prof. Tatsuya Tsukuda, Tokyo University (Japan), Toward precise control of morphology and interfacial structure of ligand-protected gold clusters

Prof. Vlasta Bonacic-Koutecky, Humboldt-Universität zu Berlin (Germany), Tuning optical and catalytic properties of ligated silver clusters by synergistic role of metallic and organic subunits

Prof. Silvana Botti, Friedrich-Schiller Universität Jena (Germany), Electronic excitations in Cu-chalcogenide and perovskite solar cell absorbers

Prof. Maria Antonietta Loi, University of Groningen (Netherlands), Colloidal Quantum Dot Solids: determination of the energy levels and tuning of the electronic properties

Prof. Arash Mostofi, Imperial College London (UK), Challenges and opportunities in large-scale electronic structure simulations

Prof. Jaakko Akola, Tampere University (Finland), Small Au nanoparticles quantum confinement effects and atomic scale simulations of interactions in biological environments

Dr. Miguel A. Caro, Aalto University (Finland), Orbital-free density functional theory: looking back to the roots of DFT

Dr. Mariana Rossi, University of Oxford (UK), Dynamics of polypeptides from first principles for electrons and nuclei (and towards metal-peptide interactions)

Prof. Jens Müller, University of Münster (Germany), DNA duplexes with silver(I)-mediated base pairs

Prof. Stephan Kümmel, Bayreuth University (Germany), Metal nano alloys – insights from DFT and insights into DFT

Dr. Elke Pahl, Massey University Auckland (New Zealand) , Mercury Clusters and the Solid: Challenges of an Ab Inito Description

Prof. Noa Marom, Tulane University (US), Toward Computational Design of Cluster-Based Functional Nano-Structures

Steven Swaswey, University of California Santa Barbara (US), Clusters with a twist: fluorescent silver clusters stabilized by DNA

Prof. Roy Johnston, University of Birmingham (UK), Combining Theory and Experiment to Determine the Structures of Sub-nanometre Metal Clusters

Dr. Olga Syzgantseva, Aalto University (Finland), Excited state charge transfer in the hybrid perylene - titanium oxide system: an ab initio study

Prof. M. Arturo López Quintela, University of Santiago de Compostela (Spain), Small metal

clusters without protecting ligands: synthesis, catalytic properties and DNA interaction

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