Thursday Afternoon, October 31, 2013

Accelerating Materials Discovery for Global Competitiveness Focus Topic
Room: 202 B - Session MG-ThA

Theory, Computation and Data-Enabled Scientific Discovery
Moderator: T. Mueller, Johns Hopkins University

2:00pm **MG-ThA1 High-throughput Quantum Chemistry and Virtual Screening for Materials Solutions**, ***M.D. Halls***, *D.J. Giesen, H.S. Kwak, A. Goldberg, T.F. Hughes, Y. Cao*, Schrödinger Inc.

For the past 20 years the standard approach to drug discovery has been the automated computational screening of chemical structure libraries to identify lead systems for further investigation and experimental development. Recent advances in the power of computational resources and the improvements in the efficiency and stability of first-principles simulation packages has made it possible to apply this paradigm to challenges in material science. It is now possible for multi-step property calculations using accurate quantum-based methods to be executed automatically for diverse chemical libraries, with the results collected in a growing data record. This record can then be sorted and mined to identify exemplary candidates and establish critical structure-property limits within a chemical design space. To date very few studies have been reported in which quantum chemical calculations are carried out in a high-throughput fashion to compute properties and screen for optimal materials solutions, however with time virtual screening will become central to advanced materials chemistry research.

In this presentation, the use of high-throughput quantum chemistry to analyze and screen a chemical structure library is demonstrated for key materials applications including organic light-emitting diode (OLED) and organic photovoltaic (OPV) materials, and precursors for optimal thin film deposition in semiconductor device fabrication.

2:20pm **MG-ThA2 Computational Materials Design: Precious Material Free Catalyst for NO Dissociation**, ***H. Kasai***, *A.A. Padama*, Osaka University, Japan

We entered the 21st Century witnessing remarkable progress in Science and Technology. Novel materials and devices that were once considered the stuffs of *science fiction* are becoming a reality. It would not be an exaggeration to say that we are coming to the **Age ofDesigner Materials**. **Complex materials** are designed to have desired properties, with both basic and technological applications. A **Designer Material** has to be **Functional**. To realize this and to test the concepts and principles developed for realizing designer materials, we use **Surfaces** as our testing ground. These give access to the appropriate reduced dimensionality and means to manipulate the degree of complexity, and emergence of function.

Specifically, we were able to design catalyst for NO dissociation that is free from precious materials. NO is emitted from the combustion of fossil fuels and converts to nitric acid in the atmosphere which leads in the formation of acid rain. The dissociation of NO is known to be the rate limiting process for its reduction due to the strong N-O bond [1]. Precious metals such as Rh, Pd and Pt are efficient catalysts for such purpose but their high cost prohibits their massive production [2]. Through first principles investigation, we were able to confirm that Cu-based surface is capable of dissociating NO molecule [3, 4]. The analysis is made with reference to a clean Cu surface. In Cu(111), dissociation of NO is accompanied by a large activation barrier and NO desorption is more likely to happen. This is due to the filled d states of the Cu atoms which limits their interaction with the adsorbate. In the contrary, the local density of states profile of the d orbital of the Cu atoms in Cu_2O(111) shows that the states are shifted to the Fermi level region which explains the good adsorption and easy dissociation of NO. We also found that the reaction path of NO on Cu_2O surface is comparable with that of Rh surface which is characterized by a transition state lying below the reference level (surface and NO_{gas}) [5]. Nevertheless, the activation barrier for NO dissociation is lower in Cu_2O indicating the easier dissociation of NO on the alternative catalyst. Furthermore, the adsorption energy of N and O atoms from the dissociated molecule is also lower on Cu_2O which is desirable for the succeeding steps in the reduction process.

References:

[1] S. Gonzalez et al., J. Catal. 239 (2006) 431.

[2] H.J. Kwon et al., Chem. Eng. Sci., 62 (2007) 5042.

[3] A.A.B. Padama et al., J. Phys.: Condens. Matter, 24 (2012) 175005.

[4] H. Kishi et al., J. Phys.: Condens. Matter, 24, 262001 (2012).

[5] H. Kasai et al., J. Jpn. Petroleum Institute, (2013) *accepted for publication.*

2:40pm **MG-ThA3 Computer-aided Design of Materials for CO_2 Utilisation**, ***N.H. de Leeuw***, Unaffiliated, *A. Roldan, N. Hollingsworth, J. Goodall*, University College London, UK **INVITED**

Despite the high thermodynamic stability of CO_2, biological systems are capable of both activating the molecule and converting it into a range of organic molecules, all of which under moderate conditions. It is clear that if we were able to emulate Nature and successfully convert CO_2 into fuel or useful chemical intermediates, without the need for extreme reaction conditions, the benefits would be enormous: One of the major gases responsible for climate change would become an important feedstock for the fuel, chemical and pharmaceutical industries!

Iron-nickel sulfide membranes formed in the warm, alkaline springs on the Archaean ocean floor are increasingly considered to be the early catalysts for a series of chemical reactions leading to the emergence of life. The anaerobic production of acetate, formaldehyde, amino acids and the nucleic acid bases - the organic precursor molecules of life - are thought to have been catalyzed by small cubane (Fe,Ni)S clusters which are structurally similar to the surfaces of present day sulfide minerals such as greigite (Fe_3S_4) and mackinawite (FeS).

Contemporary confirmation of the importance of sulfide clusters as catalysts is provided by a number of proteins essential to modern anaerobic life forms, e.g. ferredoxins or (de)hydrogenases, all of which retain cubane (Fe,Ni)S clusters with a greigite-like local structure, either as electron transfer sites or as active sites to metabolise volatiles such as H_2, CO and CO_2.

We have used a combination of computation, synthesis and electrochemistry to mimic Nature and produce Fe-S and Ni-doped Fe-S nanoparticles to catalyse the conversion of CO_2. Careful and sensitive testing of the computationally designed materials, prepared through novel synthesis routes, shows that the nanoparticles have the power to adsorb CO_2 and reduce it to formic acid - a useful chemical intermediate. A particularly promising aspect is that the catalytic conversion of CO_2 takes place at room pressure and temperature and at the sort of low voltages that could be obtained from solar energy, thus making it a sustainable process.

3:40pm **MG-ThA6 Surface Technology Solutions: Materials Design for Aero-Engine Gas Turbine Applications**, ***J.R. Rodgers***, Toth Information Systems Inc., Canada **INVITED**

Erosion damage of aero-engine compressor gas path components occurs to aircraft operating in sandy environment. Erosion can lead to gradual changes in surface finish and component geometry, which consequently alters the dynamic response characteristics of compressor airfoils, causing premature failure. One of the approaches to deal with erosion problems in gas turbine engines is to apply protective hard coating on the component surface. Hardness and ductility are two of the key values for the design and characterization of materials that are used for surface protection. These key values largely depend on the elastic properties of the material, as described by the elastic stiffness tensor. Materials informatics approaches and high-throughput c omputational materials science methods have been employed, to explore chemistry and property space, to aid the prediction, synthesis, characterization and property optimization of promising candidate materials, for protective hard coatings systems, with enhanced erosion resistance for application to gas turbine airfoils. These generic methods have been employed to explore multidimensional property space, at a previously unavailable level of detail and to rapidly calculate thermophysical properties that are difficult to measure. Given these vast resources of structure and property data it is possible to extract trends on the structure of materials and their properties and use these results at the materials selection and design stages. These informatics approaches, coupled with *ab initio* quantum mechanics methodologies, provide many of the tools needed to guide materials selection via computational experiments. Examples for the application of these methods coupled with the use of experiments for the design of materials for industrial applications will be presented. The results presented will highlight the potential of this combined – informatics, theoretical and experimental – research strategy to aid the manufacturing process.

4:20pm **MG-ThA8 Exploring Electronic Structure in the Search for New Functional Materials**, ***M. Klintenberg***, Uppsala University, Sweden **INVITED**

The Electronic Structure Project (ESP/ELSA)[1-3] is an initiative that dates back to 2001 [4,5] and today contain tens of thousands of materials that

have been investigated using robust and high accuracy electronic structure methods (all-electron full-potential linear muffin-tin orbital approach, FP-LMTO). A short history of the project, the present capabilities of ESP/ELSA including some examples of successful studies using ESP as well as future developments and outlook will be presented.

[1] http://www.materialsgenome.se (re-directed to http://gurka.fysik.uu.se/esp).

[2] A high accuracy fermi-surface database can be found at http://gurka.fysik.uu.se/esp-fs

[3] "Data mining and accelerated electronic structure theory as a tool in the search for new functional materials", C. Ortiz, O. Eriksson and M. Klintenberg. Comput. Mater. Sci. 44, 1042-1049 (2009)

[4] "A systematic search for new scintillators using electronic structure calculations", M. Klintenberg, S. E. Derenzo and M. J. Weber, Nanotech, 2, 427 (2002). Technical Proceedings of the 2002 International Conference on Computational Nanoscience and Nanotechnology, http://www.nsti.org/procs/ICCN2002/16/W62.11

[5] "Potential new scintillators identified by electronic structure calculations", M. Klintenberg, S. E. Derenzo and M. J. Weber, Nucl. Inst. Meth. A, 486, 298 (2002), http://www.sciencedirect.com/science/article/pii/S0168900202007234

5:00pm **MG-ThA10 Data-Driven Discovery of Physical, Chemical, and Pharmaceutical Materials**, ***B.A. Jones***, IBM Almaden Research Center **INVITED**

Data-driven insights have aided materials discovery in the pharmaceutical and related chemical areas for some years now, with even commercial products available. I will describe some successes in these areas, and derive lessons which might be applicable to the areas of condensed matter and polymeric materials. Three points which l will be emphasizing are that a) Just as experiment, theory, and computation must guide each other for MGI to succeed, a triangle of inter-relationships, for MGI it is really a tetrahedron, with computer science forming the fourth vertex. I will discuss the benefits which modern computer science can bring in the areas of modern data mining, machine learning, and big data analytics techniques. The volume of data on materials is fast-growing and scattered across many sources. While new tools and platforms have allowed the processing of vast volumes of data, our ability to integrate heterogeneous and unstructured data sets is still developing. The ability to correlate data from multiple sources deepens the value of data and allows new insights to emerge. b) The elements of accelerated materials discovery are different in the different scientific fields. Pharmaceutical discovery involves extracting chemical constituents and structures from patents; polymer data is scattered, unstructured, statistical and often ambiguous; and in condensed matter we tend to look at materials properties as a function of some parameter such as doping or temperature, often in graph form. Understanding the needs of both soft and hard condensed matter will help common tools and synergies to develop. c) There are many challenges ahead in fully incorporating data-enabled scientific discovery, as well as learning on both computer science and materials science sides. Getting scientific insights from both computer scientists and from data mining and databases is not yet common, and requires some work ahead in both communities to familiarize themselves with opportunities and to optimize the tools needed for future materials by design.

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