Materials Theory Group - Materials Information, Characterization, and Exploration (MTG-MICE) Summer Workshop 2013

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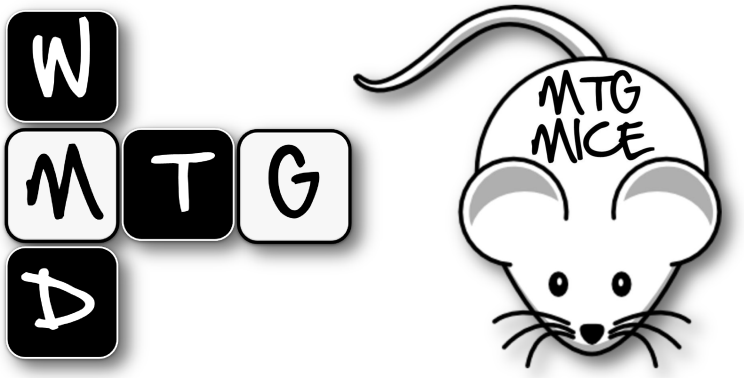

Organized by the Materials Theory Group, Yonsei University

(Michael Lee and Rachael Tak)

Joint workshop between WMD (Bath) and MTG (Yonsei)

Workshop schedule

Session 1 (Chairperson: Rachael Tak)

Time	Title	Speaker
10.00 – 10.20 AM	Towards Exascale Computational Materials Science: Challenges and Solutions	Aron Walsh (U.Bath)
10.20 – 10.40 AM	Introduction to the BRODIUM Project: Motivation and Progress	Daniel Yoo (Yonsei U.)
10.40 – 11.00 AM	Polar TiN/MgO ultrathin nanofilms	Michael Lee (Yonsei U.)
11.00 – 11.20 AM	Break / Discussion	
11.20 – 11.40 AM	From materials modelling to thin film processing: *ab initio* thermodynamics	Adam J. Jackson (U. Bath)
11.40 – 12.00 NN	Influence of *xc* functional on thermal-elastic properties of bulk ceria: A DFT-based Debye-Grüneisen model approach	Aloysius Soon (Yonsei U.)
12.00 – 12.20 PM	The TINKERBELL Project: A density-functional study of the surface phase diagram of Sn/Cu(100)	Emmanuel Yoon (Yonsei U.)
12.20 – 12.30 PM	Break / Discussion	

Session 2 (Chairperson: Michael Lee)

Time	Title	Speaker
2.00 – 2.20 PM	Pt icing on the TiN cake: An *ab initio* study	Rachael Tak (Yonsei U.)
2.20 – 2.40 PM	A vital role of materials science in a mechanical design	Bitna Lee (U. Toronto)
2.40 – 3.00 PM	An introduction to solving eigenvalue problems	Johnny Kim (Yonsei U.)
3.00 – 3.30 PM	Closing / Discussion	

Abstracts

Towards Exascale Computational Materials Science: Challenges and Solutions

Aron Walsh

Centre for Sustainable Chemical Technologies & Department of Chemistry, University of Bath, UK

High-performance computing architectures continue to rapidly evolve. In 2008, the first petascale supercomputer was built and now the first exascale systems are being commissioned, which are capable of 10^{18} floating point operations per second. The challenge in computational materials science is to efficiently exploit these massive resources.

The scaling of current materials modelling packages will be discussed (VASP, FHI-AIMS and ChemShell), in addition to strategies maximise the performance on massively parallel systems. This will include the recent implementation of k-point parallelism into the VASP code, task-farming of repetitive jobs and the importance of compiling with high-quality libraries. A number of key examples will be presented, including hydrogen dissociation at semiconductor surfaces and the band energies of TiO_2.

Introduction to the Brodium Project:

Motivation and Progress

Daniel Yoo

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Palladium nanoparticles have been widely studied due to its outstanding catalytic performance in some chemical reactions. It is found that their catalytic selectivity could be greatly enhanced via controlling the specific shape of these Pd nanoparticles. Recent papers have shown that bromide ions can be used as a capping agent to synthesize Pd nanoparticles surrounded by 100 facets (i.e. nanocubes). However, detailed atomic processes governing this morphological change is still lacking. In this work, the simulated morphology of Pd nanoparticles under a bromide ion-containing environment will be studied using density-functional theory (DFT) and the Conductor Screening Model (COSMO), as implemented in $DMol^3$ code. Specifically, the exchange-correlation functionals due to PBE and PBEsol will be used for this work. In this talk, I will present the main motivation as well as some preliminary results on chemisorded Br/Pd structures.

Polar TiN/MgO ultrathin nanofilms

Michael Lee

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Titanium nitride is classic, yet industrially important refractory material. Traditionally it has been used as durable coating material for tool tips, and has also found recent applications in multifunctional coatings. Recently, it has been successfully demonstrated that thin layers of TiN (50 nm) grow epitaxially on inert support materials like MgO substrate. Though these studies focused on characterizing the microstructure of this TiN/MgO interface, a detailed picture of both the atomic and electronic structure is still lacking. In particular, it is important to address the possible formation of ultrathin layers of polar TiN(111) at the interface, which will prove important for high-strength coating design. In this talk, I will report optimized atomic geometries of different multilayered TiN(111)/MgO(111) interface structures, and their relative energetics. Consequently, this study will provide a platform for future investigations to aid the tailoring of ultrathin TiN nanofilms for multifunctional superhard coatings in emerging technologies.

From materials modelling to thin-film processing: *ab initio* thermodynamics

Adam J. Jackson

Centre for Sustainable Chemical Technologies & Department of Chemistry, University of Bath, UK

Computational modelling with density functional theory (DFT) is an indispensable tool in the design of energy materials. However, the majority of studies focus on ground-state, zero-temperature behaviour with little direct consideration of processing issues. By calculating phonons and incorporating data for other reactants and products, it is possible to explore the operating envelopes for industrial processing.

Kesterite materials such as Cu_2ZnSnS_4 (CZTS) can form effective thin-film absorber layers for photovoltaics, while minimising or avoiding the use of rare elements. This gives them the potential for scale-up on a Terawatt scale, making a meaningful contribution to global energy needs. Many reactions have been proposed and experimentally demonstrated for the formation of CZTS. For industrial-scale deposition of films, a reaction system would ideally involve solution processing at modest temperature and pressure while avoiding rare or toxic materials.

Reaction equilibria are modelled with *ab initio* thermodynamics: energies are modelled using DFT with the PBEsol generalised gradient approximation (GGA) as implemented in FHI-aims, a quantum chemistry code which scales across thousands of cores. The harmonic approximation, using the 'direct method', is employed for temperature-dependent potentials with the Phonopy package.

Influence of *xc* functional on thermal-elastic properties of bulk ceria: A DFT-based Debye-Grüneisen model approach

Aloysius Soon

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For high-temperature applications, the chemical stability, as well as the mechanical integrity of the oxide material used is of utmost importance. Solving these problems demands a thorough and fundamental understanding of their thermal-elastic properties. In this work, we report density-functional theory (DFT) calculations to investigate the influence of the *xc* functional on specific thermal-elastic properties of bulk ceria CeO_2. Namely, we consider the local-density approximation (LDA), the generalized gradient approximation due to Perdew, Burke, and Ernzerhof (GGA-PBE), as well as a recently popularized hybrid functional due to Heyd-Scuseria-Ernzehof (HSE06). In addition, we will also report DFT+U results where we introduce a Hubbard U term to the Ce $4f$ states. Upon obtaining the DFT total energies, we then couple this to a volume-dependent Debye-Grüneisen model to determine the thermodynamic quantities of these oxides at arbitrary pressures and temperatures. We find an explicit description of the strong correlation (e.g. via the DFT+U approach and using HSE06) is necessary to have a good agreement with experimental values.

The TinkerBell Project: A density-functional study of the surface phase diagram of Sn/Cu(100)

Emmanuel Yoon

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Layer deposition of Sn on Cu(100) can give rise to a rich variety of surface reconstructions in the submonolayer surface coverage range of Sn. To date, the explicit atomic geometry of high surface coverage structure of Sn/Cu(100) is still strongly debated. Thus, using density-functional theory coupled with the *ab initio* atomistic thermodynamics approach, I hope to map out the *ab initio* surface phase diagram of the Sn/Cu(100) system, hopefully providing insight into the rich surface chemistry of this near-surface alloy system. In this talk, I will attempt to present preliminary data on bulk Sn and Cu, as well as some convergence tests performed for the clean Cu(100) surface. This will set the platform for future Sn/Cu surface alloy structure calculations.

Pt icing on the TiN cake: An *ab initio* study

Rachael Tak

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Yonsei University, Seoul 120-749, Korea

Platinum is indeed one of the most broadly used catalyst for many important chemical reactions (e.g. oxygen reduction reaction). Although it is has the much desired catalytic properties, Pt-based catalysts have not met an enthusiastic reception from the industry due to the high escalating cost of Pt. Nanoparticles of Pt deposited on C-based supports catalyst have been widely used to attempt to overcome this problem, but it is still considered as an imperfect solution because of its bad stability and durability in oxidative and acidic fuel cell conditions. In our previous work, we have found an effective way to anchor and secure single Pt atoms on a hard, durable and conductive metal nitride (TiN) support. Here we hope to study and investigate the stability and electronic structure of ultra-small Pt clusters and ultra-thin Pt monolayers on the TiN support, as an effort for reduce Pt loading.

A vital role of materials science in a mechanical design

Bitna Lee

Department of Mechanial Engineering,

University of Toronto, Toronto, Canada

In a subjective point of view of myself, who studies in mechanical engineering at University of Toronto now works as an intern in the Material Theory group under Professor Aloysius. I found that materials engineering strongly correlates with mechanical engineering since the process and selection of materials play a key role in mechanical design and development. Therefore, a close relationship between materials and mechanical engineering will be discussed in this talk. To adopt materials science approaches in mechanical design, I have chosen to study DFT (Density-Functional Theory) and EOS (Equation-of-State). Gibbs free energy-Temperature graphs of materials (i.e. fcc, hcp aluminum and fcc, hcp titaninum) will be produced based on the Energy-Volume graphs of these materials via the GIBBS2 program. This work encourages cooperation between a mechanical engineer and a materials engineer, which might take the human race to an advanced world.

An introduction to solving eigenvalue problems

Johnny Kim

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Scientific code reduces our effort to calculate numerous challenging problems. Kohn-Sham density-functional problems related to finding ground state energy have been rigourously tackled by well-written scientific code such as DMol^3 or VASP, and so on. In fact, density-functional theory calculations are delicately weaved sets of eigenvalue problems, staged for each iteration. Most of the calculations are numerically done within the program code, not shown simply to many users. Although running the program or code is certainly convenient these days, it is still beneficial for us to know what is actually going on in the algorithms. As a first step to understanding the explicit solution to Kohn-Sham density-functional theory problems, I will present an introductory presentation on how to solve eigenvalue problems using common scientific languages, such as Python, Fortran or C++.