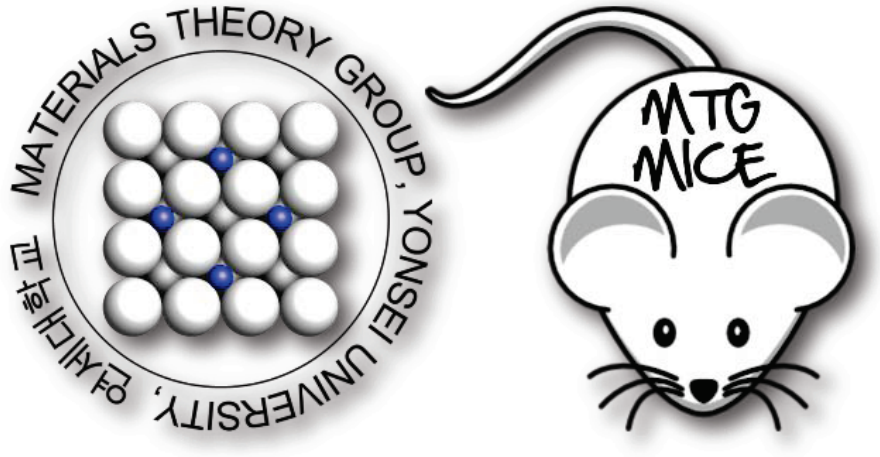
Materials Theory Group - Materials Information, Characterization, and Exploration (MTG-MICE)

1st Winter Workshop 2013

Sokcho, Gangwon-do, Korea, February 18th – 19th 2013



Organized by the Materials Theory Group, Yonsei University

(Collins Lee and Daniel Yoo)

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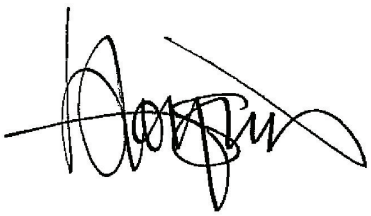
Welcome Message

Welcome to the inaugural Materials Theory Group - Materials Information, Characterization, and Exploration (MTG-MICE) 1st Winter Workshop 2013. The aim of this internal workshop series is to provide a platform for young researchers (undergraduate students, graduate students, and postdoctoral researchers of MTG) to introduce, learn and discuss the use of *ab initio* electronic structure theory in the various areas of advanced materials (electronic, magnetic and optical devices, sensors, catalysts and hard coatings). First-principles electronic structure calculations are used in conjunction with high performance computing to probe chemical reactions at interfaces and explore the energetics, atomic, electronic, and magnetic properties of these advanced materials. Young researchers are given the chance to present their latest work, as well as to initiate intra-group and international collaborations between our global partners. A special thanks to all those who have worked hard in putting this all together, especially to Mr. Collins Lee and Mr. Daniel Yoo - the main organizers for this 1st Winter Workshop in 2013.



Aloysius Soon, Ph.D.

Materials Theory Group,

Department of Materials Science and Engineering,

Yonsei University, Seoul, Korea

[Session A Nanocatalysis 1:00 PM]

A first principle study on atomic, electronic, and phononic structure of cuprous oxide

Chang-Eun Kim

Department of Materials Science and Engineering,

Yonsei University, Seoul 120-749, Korea

The copper oxide system has been widely studied extensively due to its outstanding properties in catalysis, corrosion and high-performance materials. Cuprous oxide (Cu_2O) is a well known photocatalyst for water spliting to H_2 and O_2 under visible light. The main objective here is the chemical interaction between cuprous oxide and chemical species related to the reaction, e.g. water molecule, promoters, poisons and other potential reactants. As a first step toward understanding principles behind chemical reactions on cuprous oxide surface, here we begin with *ab-initio* calculations on cuprous bulk system. We study and report the atomic structure, electronic states and phonon dispersion properties of the cuprous oxide system.

[Session A Nanocatalysis 1:20 PM]

First-principles study of surface reconstruction in CeO_2(100)

Edward Kwak

Department of Materials Science and Engineering,

Yonsei University, Seoul 120-749, Korea

In this study, we present the periodic density functional theory (DFT) calculation of bulk CeO_2 and (100) surface, which is one of the low index surfaces, to research about surface reconstruction as the change of oxygen coverage. All the calculations are performed by DFT + U methodology($U = 5$ eV) to improve the description of the strongly correlated cerium $4f$ states. Most bulk properties are well-matched with experimental information and other theoretical results, except a bulk modulus. The surface energies, corresponding to each oxygen coverage surfaces, are analyzed in function of oxygen chemical potential. The electronic properties of the surface are also analyzed by means of the electronic density of states and the electron density as the change of oxygen coverage. STM images of the (100) surface are visualized using partial charge density and compared with experimental result to identify the unit cell of reconstructed surface. We find that there are discrepancies between our theoretical result and experimental data.

[Session A Nanocatalysis 1:40 PM]

First principles study of ultrathin ceria films on copper-nickel alloys

Collins Lee

Department of Materials Science and Engineering,

Yonsei University, Seoul 120-749, Korea

To achieve higher catalytic performance of ceria on copper system, surface engineering techniques such as ad-atoms, doping, and alloys have been considered promising solutions for creating surfaces with desired chemical and physical properties. Recently, it is reported that strong enhancement of chemical reactivity by defects located at the oxide-metal interface for ultrathin MgO films deposited on Ag substrate, proposing new guiding rule for rational design of a heterogeneous catalyst. In this work, we perform density-functional theory (DFT) calculations to investigate the thermodynamic stability and electronic structure of the ultrathin ceria films on copper-based alloys (solute: Ni) as a function of concentration of solute. Also, we consider the implementation of DFT + U where we introduce a strong intra-atomic interaction (termed as the Hubbard U) in a screened Hartree-Fock like manner, as an on-site treatment to the Ce $4f$ states in ceria. We find the catalytic activity of ultrathin oxide films system grown on metal substrates can be tuned by the alloying effect to metal substrate.

[Session A Nanocatalysis 2:00 PM]

First-principles study of oxygen reduction reaction (ORR) on defective titanium nitride supported single platinum atom

Youngjoo Tak

Department of Materials Science and Engineering,

Yonsei University, Seoul 120-749, Korea

PEMFCs are labor at commercialization due to high cost though it's low operating temperature and high applicability. The biggest reason for its high cost is Platinum catalyst. So, it brought many scientists to research for reduce cost of Pt catalyst and enhance its reactivity, but clear solution has not discovered yet. In this work, I performed DFT calculation to investigate mechanism of oxygen reduction reaction (ORR) at Pt atom on defective titanium nitride (TiN) surface, which is one of the most promising materials to substitute Pt/carbon catalyst. From this study, we can find whether TiN is effective support for Pt catalyst or not. We can also find out details of ORR pathway on Pt/TiN catalyst system. Both direct pathway and series pathway of ORR are investigated.

[Session A Nanocatalysis 2:20 PM]

Computational-based catalyst design for thermochemical transformations

Emmanuel Yoon

Department of Materials Science and Engineering,

Yonsei University, Seoul 120-749, Korea

Nowadays, our society faces a decrease in the availability of conventional fossil fuels and this critical shortfall affects our globalized and industrialized world. Moreover, the excessive emission of carbon dioxide via industrial processes has accelerated much intensive research on alternative/sustainable energy sources. The main objective of this review article is to provide an overview of computational methods and advances in the rational design of catalytic materials for our modern world. Here, the discoveries of active catalysts (e.g. bimetallics) will be presented, and various adsorption models will be discussed to account for the nanoscale physio-chemical attributes of these nanocatalysts, e.g. their anisotropies, size- and shape-effects, surface coordination number and cuvature angle, etc. Worthy of mention, these studies were calculated using various levels of electronic structure theory, namely density-functional theory (DFT), addressing adsorption strength and activation barriers for these catalytic reactions. This review article will be used as a first-step in our study of active and selective nanocatalysts for novel energy-related technologies.

[Session B Nanomechanics 3:00 PM]

Charge-density distribution and electron localization function (ELF): Application to the cubic crystal structure under anisotropic strains

Michael Lee

Department of Materials Science and Engineering,

Yonsei University, Seoul 120-749, Korea

To date, the diamond-structure, composed of carbon, silicon, and germanium, are reported for a local phase transition under the high hydrostatic pressure. Also there are many reports that studied with ab initio molecular dynamics of the graphtization of flat diamond (111) surface.In this work, we attempted to survey and calculate the uniaxial stress-strain constitutive relations of the diamond structure using first-principles density-functional theory (DFT) as implemented in the the Vienna *Ab initio* Similation Package(VASP) code. By using valence charge density come from DFT calculation that are performed using the generalized gradient approimation(GGA) to the exchange-correlation potential due to Perdew,Burke and Ernzerhof(PBE) as implementerd within the VASP, we draw the charge density distribution and electron localization function(ELF) that was introduced by Becke and Edgecombe. From the ELF, the distribution of electrons between atoms in strained system show the process of change in increasing strain system.

[Session B Nanomechanics 3:20 PM]

Mechanical property of W and its improvement of hardness by using other materials

Woosun Jang

Department of Materials Science and Engineering,

Yonsei University, Seoul 120-749, Korea

In this work, we studied about mechanical property of W and its hardness-improvement by using VASP(Vienna Ab-initio Simulation Package), which can perform ab-initio simulations, to obtain datas including energies. The hardness of material can be increased by alloying or planting other materials into its layer to provide defects, which blocks grain boundaries from moving. This phenomenon strengthens the materials(Hall-petch relation). To observe these processes, at first, we calculated many mechanical constants of pure W and Al-implanted structure including bulk and shear modulus with VASP. Next, we observed mechanical properties of each structures based on calculated constants. Then, we compared two properties to find differences between two properties. Also, we followed the same steps above with implanting other materials, and compared the improvement of mechanical properties with the improvements given by Al-implantation.

[Session C Nanoelectronics/Nanoinformatics 3:40 PM]

The practical introduction to hybrid functional with Si and Zn_3N_2 as examples

Daniel Yoo

Department of Materials Science and Engineering,

Yonsei University, Seoul 120-749, Korea

First-principles calculation based on density-functional theory is the main tool to analyze various properties of materials. Even though conventional DFT such as LDA or GGA have been actively applied in the research area, the electronic properties obtained by these fuctionals have quite huge error comparing with experiments. In order to overcome these limitation, the hybrid method have been suggested through the combination of DFT and HF theory. One of hybrid functionals proposed by Heyd-Scuseria-Ernzerhof, HSE06, shows the good agreement in the various materials systems. In this work, the practical way to use HSE06 fuctional is introduced in terms of investigating the band structure, density-of-states, partial charge density of silicon and zinc nitride. Besides, it can be advanced to the way to plot the optical absorption if the calculation is successful. Through this work, not only the investigation of silicon can be a tutorial for exercising of HSE06 calculation, but also zinc nitride results can show the practical example of the hybrid fuctional.

[Session C Nanoelectronics/Nanoinformatics 4:00 PM]

Introduction about GPU computing and the possibility of VASP calculation faster using GPU

Jaehwan Jung

Department of Materials Science and Engineering,

Yonsei University, Seoul 120-749, Korea

For long time, GPU(Graphic Processing Unit) is only used for caculating graphics. Not like CPU, which has few big and fast cores, GPU has hundreds of little and slow cores. That make GPU extremly specialized into parallelized computation like graphics, matrix and fourier transformation, etc. Lately, people try to use GPU for caculation not only for graphical usages, and it become going well. VASP, ab-initio simulation program, based on DFT, which has constructed mostly by parallelisable caculations. Programming to use GPU is not simple. especially distribute operations and datas to each cores. Bad code make caculation even slower when using more number of core. Some teams already tried VASP calculation by GPU. They got results that 1CPU + 1GPU caculate 2 to 20 times faster then using single CPU. PROF.DR. M.T.M. KOPER at Leiden Institute of Chemistry (UL) do project to make GPU version of VASP now. If we run VASP with GPU successfully, it will be very helpful to all of us, both money and time.