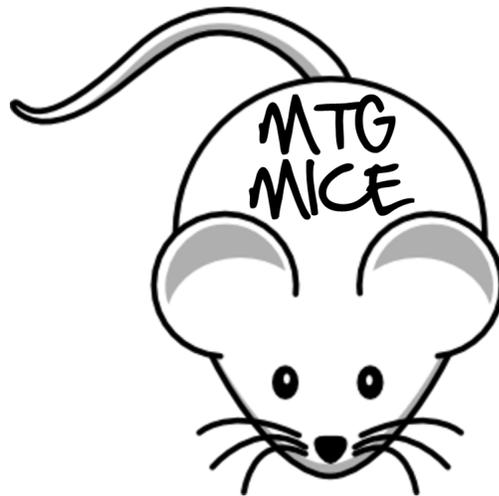
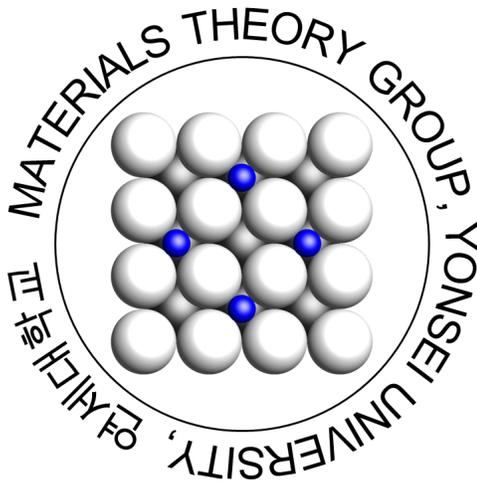


Workshop in 2015

The 5th Materials Information,
Characterization, and Exploration
(MICE-5)

B417, Engineering Building B, Yonsei University,
Seoul, Korea

January 12th Monday 2015



Organized by Materials Theory Group, Yonsei
University, Korea

Workshop schedule

(Every talk consists of 12 min talk and 8 min Q&A)

Time	Title	Speaker
10:00 ~ 10:10	Introduction of MICE-5 in 2015	Jongmin Yun
10:10 ~ 10:20	Opening announcement	Aloysius Soon
Session I : Compound material (Chairman : Jongmin Yun)		
10:20 ~ 10:40	How are your course? # 2	Su-Hyun Yoo
10:40 ~ 11:00	A DFT study of oxygen reduction reaction on single-atom Pt nanocatalyst	Youngjoo Tak
11:00 ~ 11:20	Study of the stoichiometric diversities of TiN_x	Yong-Hyuk Lee
11:20 ~ 11:40	Effect of gold subsurface layer on the surface activity and segregation in Pt/Au/Pt ₃ M (where M = 3d transition metals) alloy catalyst from first-principles	Chang-Eun Kim
Lunch break (100min)		
Session II : Adsorption phenomena & functional (Chairman : Su-Hyun Yoo)		
13:20 ~ 13:40	Oxygen adsorption on metal system	Ji-Hyun Lim
13:40 ~ 14:00	Surface oxide effect on the adhesion of PMDA-ODA on Cu(111)	Jong-Hun Park
14:00 ~ 14:20	Change of binding energy between Cu(110) and halogen atoms as a function of binding sites	Young-Kwang Jung
14:20 ~ 14:40	Influence of van der Waals corrected xc -functionals on the anisotropic mechanical properties of coinage metals	Ji-Hwan Lee
Coffee break (20min)		
Session III : 2D material (Chairman : Ji-Hwan Lee)		
15:00 ~ 15:20	Grain boundaries in Phosphorene and MoS ₂	Kisung Kang
15:20 ~ 15:40	Properties of MXene, depending on environment	Jongmin Yun
15:40 ~ 16:00	Electronic and optical properties of ultrathin silicon nanosheets : A first-principles investigation	Woosun Jang
16:00 ~ 16:20	Closing announcement	Aloysius Soon

Abstracts

- (1) [Session I : Compound material]
How are your course? # 2
by Su-Hyun Yoo 4
- (2) [Session I : Compound material]
A DFT study of oxygen reduction reaction on single-atom Pt nanocatalyst
by YoungJoo Tak 5
- (3) [Session I : Compound material]
Study of the stoichiometric diversities of TiN_x
by Yonghyuk Lee 6
- (4) [Session I Compound material]
Effect of Gold Subsurface Layer on the Surface Activity and Segregation
in Pt/Au/ Pt_3M (where M = 3d transition metals) Alloy Catalyst from
First-Principles
by Chang-Eun Kim 8
- (5) Session II : Adsorption phenomena & functional]
Oxygen adsorption on Metal system
by Ji-Hyun Lim 9

- (6) [Session II : Adsorption phenomena & functional]
Surface oxide effect on the adhesion of PMDA-ODA on Cu(111)
by Jonghun Park 10
- (7) [Session II: Adsorption phenomena & functional]
Change of binding energy between Cu(110) atoms and halogen atoms as
a function of binding sites
by Young-Kwang Jung 12
- (8) [Session II : Adsorption phenomena & functional]
Influence of van der Waals corrected *xc*-functionals on the anisotropic
mechanical properties of coinage metals
by Ji-Hwan Lee 13
- (9) [Session III : 2D material]
Grain boundaries in Phosphorene and MoS₂
by Kisung Kang 14
- (10)[Session III : 2D material]
Properties of MXene, depending on environment
by Jongmin Yun 15
- (11)[Session III : 2D material]
Electronic and optical properties of ultrathin silicon nanosheets: A first-
principles investigation
by Woosun Jang 17

Session I : Compound material 10:20 - 10:40

How are your course? # 2

Su-Hyun Yoo

Department of Materials Science and Engineering,

Yonsei University, Seoul 120-749, Korea

Collins gave a talk "*How are your course?*" in March 2013, regarding motivations and plan of his course with guiding other members to their courses simultaneously. The talk was conducive to designing my degree course because it began at the right time. As one of people who have taken advice from the talk, I believe that the second version of "*How are your course?*" based on my MTG experience would be helpful for some of members to obtain the same things. In this talk, what I have learned from conducted projects (Zn_3N_2 , Brodium, CdTe and EPP) will be presented, focusing research tips. Additionally, some of important principles in the degree course and lab life will be discussed.

Session I : Compound material 10:40 - 11:00

A DFT study of oxygen reduction reaction on single-atom Pt nanocatalyst

Youngjoo Tak

*Department of Materials Science and Engineering,
Yonsei University, Seoul 120-749, Korea*

Platinum is one of the most broadly used catalyst for many chemical reactions (e.g. oxygen reduction reaction). Although its great reactivity, platinum catalysis has not met enthusiastic reception from industry due to its high price. Pt/C catalyst is widely used to come over this problem, but still considered as an imperfect solution because of its poor stability [1,2]. Recently, platinum single-atom catalyst with TiN support has suggested and proved to be stable on the N vacancy site of TiN support under N-lean condition [3]. In this work, we present density-functional theory (DFT) study of the oxygen reduction reaction on single Pt atom embedded on the surfaces of TiN(100) within the computational hydrogen model (CHE) [4].

- [1] Z. Peng *et al.*, *Nano Today***4**, 143 (2009)
- [2] B. Avasarala *et al.*, *J. Mater. Chem.***19**, 1803 (2009)
- [3] R. Q. Zhang *et al.*, *Phys. Chem. Chem. Phys.* **14**, 16552 (2012)
- [4] Nørskov *et al.*, *J. Phys. Chem. B* **108**, 17886 (2004)

Session I : Compound material 11:00 - 11:20

Study of the stoichiometric diversities of TiN_x

Yonghyuk Lee

Department of Materials Science and Engineering,

Yonsei University, Seoul 120-749, Korea

In Titanium nitride, nitrogen vacancies, V_N are regarded as the primary defects that control the composition ratio of sub-stoichiometric TiN [1]. However, the effect of nitrogen condition to the TiN system still remains an open question. According to this curiosity, in previous talk, I suggested several predicted structures of TiN_x in N-lean or N-rich condition which is Ti_2N or Ti_3N_4 . In the paper by V. Ivashchenko and *et al.*, they suggest several stable or meta-stable phases of Ti_2N which can be represented in ϵ - Ti_2N , δ' - Ti_2N , and Cd_2I -type phase. On the other hands, the paper written by P. Kroll [3] revealed that Ti_3N_4 has not only the orthorhombic Zr_3N_4 -type structure but also the cubic Th_3P_4 -type phase. With the suggested phases from the papers, I did the various understandings about a paper [4] as a methodology for bulk phase study in this talk as a first step toward my goal of the year plan. The paper suggests a bunch of approaching methods to an unknown material. This study may hopefully give generous understandings about the stoichiometric phases of TiN_x .

[1] Z. Dridi *et al.*, *J. Phys. : Condens. Matter* **14** 10237 (2002)

[2] V. Ivashchenko *et al.*, *Phys. Rev. B* **86**, 064109 (2012)

[3] P. Kroll, *Phys. Rev. Lett.* **90**, 125501 (2003)

[4] H. Xiang *et al.*, *J. Eur. Ceram. Soc.*, **34** 1809 (2014)

Session I : Compound material 11:20 - 11:40

Effect of Gold Subsurface Layer on the Surface Activity and Segregation in Pt/Au/Pt₃M (where M = 3d transition metals) Alloy Catalyst from First-Principles

Chang-Eun Kim, Dong-Hee Lim, Jong Hyun Jang, Hyoung Juhn Kim, Sung Pil Yoon, Jonghee Han, Suk Woo Nam, Seong-Ahn Hong, Aloysius Soon, and Hyung Chul Ham

Department of Materials Science and Engineering,

Yonsei University, Seoul 120-749, Korea

The effect of a subsurface hetero layer on the activity and stability of Pt skin layer of Pt₃M core-shell catalyst have been investigated using the spin-polarized density functional theory calculation. First, we find the interaction between the Pt skin surface and the gold subsurface can significantly modify the electronic structure of the Pt skin surface in Pt/Au/Pt₃M system. In particular, the local density of states projected onto the *d* states of Pt skin surface near the Fermi level is drastically decreased compared to the Pt/Pt/Pt₃M case, leading to the reduction of the oxygen binding energy of the Pt skin surface. Furthermore, a subsurface gold layer is found to cast the energetic barrier to the segregation loss of metal atoms from the bulk (inside) region, which can enhance the durability of Pt₃M based catalytic system in oxygen reduction condition at fuel cell devices.

Session II : Adsorption phenomena & functional 13:20 - 13:40

Oxygen adsorption on Metal system

Ji-Hyun Lim

Department of Materials Science and Engineering,

Yonsei University, Seoul 120-749, Korea

Understanding the interaction between oxygen and metals is important for improving materials to deal with corrosion and catalysis, etc. Also, anode metals in promising metal-air batteries, can react with air oxygen and can make oxide structures. For this reasons, investigation of oxide formation and oxide structure are necessary.

First part of this talk is chemisorption of oxygen on Mg surface, which shows unsimilarity with well understood late transition metals in terms of oxygen-oxygen interactions. Binding energy of oxygen on various surface and subsurface Mg sites is calculated using first-principles density functional theory (DFT). Interaction of oxygen-oxygen is also investigated and based on attractive oxygen-oxygen interaction, modelling of oxygen cluster formation, growth and oxide nucleation also will be discussed.

Second part will be the interaction between oxygen and Zn surfaces which is calculated with various coverage using DFT, inspiring by work done on Mg. Generally binding energies are decreased as increasing coverage, and large reconstruction was observed on several cases. This reconstruction thought to be an initial stage of ZnO formation

Session II : Adsorption phenomena & functional 13:40 - 14:00

Surface oxide effect on the adhesion of PMDA-ODA on Cu(111)

Jong-Hun Park

Department of Materials Science and Engineering,

Yonsei University, Seoul 120-749, Korea

As the increase of the attention on the flexible printed circuit board (FPCB), poly(pyromellitic dianhydride oxydianiline) (PMDA-ODA) has taken center stage among the polyimides because of high flexibility, good mechanical strength, and high thermal and chemical resistance. However, the poor adhesion of the interface between metal and PMDA-ODA coming from the surface properties of PMDA-ODA makes limitation for the usage as FPCB materials. There have been the investigations in order to overcome the poor adhesion of metal/PMDA-ODA interface by increasing surface roughness, inserting interlayer, and plasma and ion beam treatments. Even though plasma and ion treatment brought the great improvement of the adhesion by cutting molecular bonds of the PMDA-ODA and generating the functional groups in the interface and the roughness of it, there still are some limitations.

Cu(111) surface oxide layer has been studied for the catalytic application. From these studies, it unfolded that the $p(4 \times 4)$ surface oxide structures on Cu(111) are thermodynamically stable in the surface oxide state. The unique honeycomb surface structure of the $p(4 \times 4)$ surface oxide structure and the existence of the oxygen in it correspond the increase of the surface roughness and the functional groups in the trial for the improvement of the metal/polyimide adhesion. In this study, therefore, we will investigate the adhesion

of PMDA-ODA on the $p(4 \times 4)$ surface oxide structure of Cu(111) by comparing with the case of the pristine surface.

Session II : Adsorption phenomena & functional 14:00 - 14:20

Change of binding energy between Cu(110) atoms and halogen atoms as a function of binding sites

Young-Kwang Jung

Department of Materials Science and Engineering,

Yonsei University, Seoul 120-749, Korea

Nanocrystals are fundamental to modern science and technology [1]. For metal nanocrystals, the shape determines their technological relevance for catalytic, plasmonic, photonic, and electronic applications as well as their physicochemical properties [2]. In this work, we present density-functional theory (DFT) study to investigate morphology change of coinage metal (Cu, Ag, and Au) nanocrystals in various halogen (F, Cl, Br, and I) environment. Based on DTF calculation data [3], we applied *ab initio* atomistic thermodynamics theory (*aiAT*) to check thermodynamic stability of each halogen/coinage metal system [4]. After that, we predict equilibrium crystal shapes (ECS) of copper in F, Cl, Br and I environment, respectively, by employing Gibbs-Wulff shape theorem.

[1] Y. Xia *et al.*, *Angew. Chem. Int. Ed. Engl.* **48**, 60 (2009)

[2] A. Ruditskiy *et al.*, *MRS Bulletin* **39**, 727 (2014)

[3] A. Migani *et al.*, *J. Phys. Chem. B* **110**, 11894 (2006)

[4] K. Reuter *et al.*, *Handbook of Materials Modeling* (Springer, Berlin, 2005), Vol. 1.

Session II : Adsorption phenomena & functional 14:20 - 14:40

**Influence of van der Waals corrected xc -functionals on the
anisotropic mechanical properties of coinage metals**

Ji-Hwan Lee

Department of Materials Science and Engineering,

Yonsei University, Seoul 120-749, Korea

Current materials-related calculations employ the density-functional theory (DFT), commonly using the (semi-)local-density approximations for the exchange-correlation (xc) functional. The accuracy to studying the electronic structure depends not only on the employed approximation to the xc potential but also upon the system which is being investigated. The difficulties in arriving at a reasonable description of van der Waals (vdW) interactions by DFT-based models, is to date a big challenge. This stems from the well-known fact that vdW interaction is a non-local correlation effect which is not captured in the deployed (semi-)local xc functionals. In this work, using various flavours of vdW-corrected DFT xc functionals, we study the lattice and mechanical properties (including the elastic constants and anisotropic stress-strain curves) of the coinage metals (copper, silver, and gold), and critically assess the reliability of the different vdW-corrected DFT methods in describing their anisotropic mechanical properties which are less reported on in the literature.

Session III : 2D material 15:00 - 15:20

Grain boundaries in Phosphorene and MoS₂

Kisung Kang

Department of Materials Science and Engineering,

Yonsei University, Seoul 120-749, Korea

Interfaces such as grain boundary are site for mechanical failure, chemical reaction, segregation of impurities, nucleation and rapid diffusion. It is common in bulk metal, ceramic and even 2-D materials such as graphene, h-BN[1], phosphorene and MoS₂. Because of the complex structure of phosphorene and MoS₂, there are diverse candidates of grain boundary. We define the grain boundary in 2-D material by two ways; stacking fault and growth fault. Based on that, for phosphorene there are four kinds of starting structures (4:8p, 4:8c, 4:4s and 4:4t), while MoS₂ has two starting structures (4:8 and 4:4). Those structures can be changed and become different structures after relaxation.

[1] A. Singh and U. V. Waghmare, *Phys. Chem. Chem. Phys* **16** 21664 (2014)

Session III : 2D material 15:20 - 15:40

Properties of MXene, depending on environment

Jongmin Yun

*Global E³ Institute and Department of Materials Science and Engineering,
Yonsei University, Seoul 120-749, Korea*

Although tremendous interest in 2D materials, there are only relatively few freestanding monolayer materials achieved in experiments. The first example was graphene. After that, inorganic layered materials, complex oxides, metal coordination polymers, polymeric Fe-phthalocyanine have also been isolated as 2D single sheets via mechanical separating and chemical exfoliation or have been grown on substrate surface through CVD. [1]

Recently, MXene have been started to be focused as new freestanding 2D material. The exfoliated 2D carbide and carbonitride nanosheets are named as MXene to accent their structural similarity to graphene. The synthesis and exfoliating can be done by etching the MAX powder and sonicating it. Furthermore, recent research about massive delamination of MXene with intercalation has been reported. There is only one experimental case with intercalation. $\text{Ti}_3\text{C}_2(\text{OH})_2$ is intercalated with hydrazine (N_2H_4) and it is sonicated in dimethylsulfoxide (DMSO) very easily. [2]

However, the understanding about monolayer MXene and terminating system in theoretical field with respect to some variables is not fully dealt with.[3] In this talk, we will discuss the significant variables for investigating MXene properties and the variable stability depending on environment based on literature review and so on.

- [1] Qing Tang, *et al.*, *J. Am. Chem. Soc.* **134**, 16909 (2012)
- [2] O. Mashtalir, *et al.*, *Nat. Commun.* **4**, 1716 (2013)
- [3] M. Naguib, *et al.*, *Adv. Mater.* **26**, 992 (2014)

Session III : 2D material 15:40 - 16:00

**Electronic and optical properties of ultrathin silicon nanosheets:
A first-principles investigation**

Woosun Jang

*Global E³ Institute and Department of Materials Science and Engineering,
Yonsei University, Seoul 120-749, Korea*

Owing to its unique and exotic physical and chemical properties, there has been a lot of effort undertaken to explore and study ultrathin low-dimensional nanostructures (e.g. graphene and MoS₂) [1-2]. Of late, two-dimensional (2D) nanomembranes of silicon a well-known prototypical bulk semiconductor have attracted much attention, and has found its potential in niche nanodevice applications e.g. field effect transistors (FET) and secondary battery anodes [3-4]. In this work, after considering various nanomembranes of Si with varying thicknesses, we study geometric and electronic structures using first-principles density-functional theory calculations (and beyond). Here, we consider both bulk-terminated pristine Si nanomembranes as well as surface-reconstructed ones, as motivated by available experimental and theoretical reports [5-6]. To understand the influence of growth conditions on these Si nanomembranes, we have also studied the role of surface-passivation (e.g. with O, H, and OH) on their electronic and optical properties. Namely, we carefully investigate their thickness-dependent electronic band structure (i.e. both their fundamental and optical band gap energies), so as to elucidate their intrinsic structure-property relations for designing future technologically important nanodevices.

- [1] A. Geim, K. Novoselov, *Nat. Mater.* **6**, 183 (2007)
- [2] K. Kim, Y. Zhao, H. Jang *et al.*, *Nature* **457**, 706 (2009)
- [3] T. Miyazaki, T. Kanayama, *Appl. Phys. Lett.* **91**, 082107 (2007)
- [4] H. Okamoto *et al.*, *J. Am. Chem. Soc* **132**, 2710 (2010)
- [5] H. Jang, W. Lee, S. M. Won *et al.*, *Nano Lett.* **13**, 5600 (2013)
- [6] T. Morishita, M. J. S. Spencer *et al.*, *Chem. Phys. Lett.* **506**, 221 (2011)