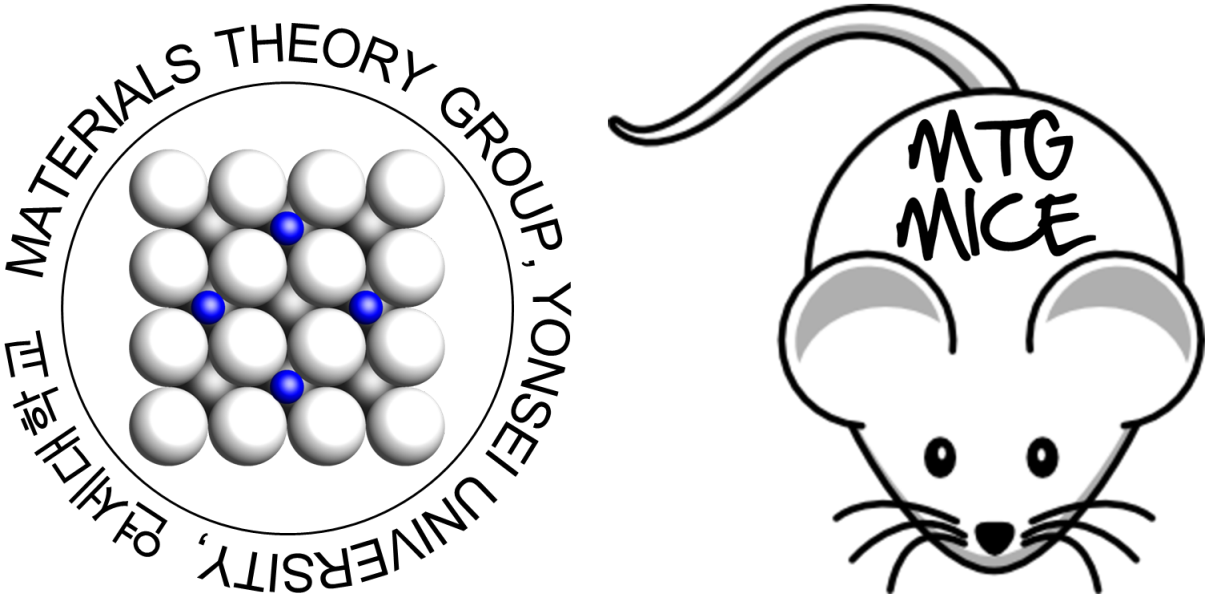
Materials Information, Characterization, and Exploration

(MICE)

Spring Workshop 2014

March 15th 2014



Organized by Materials Theory Group, Yonsei University, Korea

Workshop schedule

Time	Title	Speaker
10:00 ~ 10:10	Introduction of MICE 2014 Spring	Woosun Jang John Jonghun Park
10:10 ~ 10:20	Opening announcement of A. Soon	Aloysius Soon
Electronics and transport phenomena		
10:20 ~ 10:50	Ultrafast carrier dynamics in graphene	Torben Winzer
10:50 ~ 11:15	First principles investigations on nano materials	Johnny Changeun Kim
11:15 ~ 11:40	Study of semiconducting and metallic 2D compounds	Woosun Jang
Lunch Break		
Catalysis and energy materials		
13:00 ~ 13:30	Effects of Doping on the Concentrations of Defects at Metal-Oxide Surfaces	Norina Richter
13:30 ~ 13:55	Magic to stabilize intermediate surface structures of ceria on reduced CeO_2:A first-principles investigation	Collins Taehun Lee
13:55 ~ 14:20	TiN, Pt, MTG and Me	Rachael Youngjoo Tak
Intermission		
Morphology and surface thermodynamics		
14:40 ~ 15:05	The introduction to Su-Hyun's research themes	Daniel Suhyun Yoo
15:05 ~ 15:30	What Michael have been studied	Michael Jihwan Lee
15:30 ~ 15:55	DFT study of surface alloy of Sn/Cu(100)	Emmanuel Jongmin Yun
15:55 ~ 16:20	Wetting and the effect	John Jonghun Park
16:20 ~ 16:30	Closing announcement of A. Soon	Aloysius Soon
16:30 ~	Extra discussion time	MTG members

Abstracts

[Team 3]

Ultrafast carrier dynamics in graphene

Torben Winzer

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A microscopic theory on the ultrafast relaxation dynamics of optically excited carriers in graphene is presented.

Based on the density matrix formalism and applying tight-binding wave functions, the carrier dynamics is resolved in momentum space and time. Accounting for the electron-light interaction as well as many-particle contributions such as electron-phonon and electron-electron scattering, the presented approach offers a realistic description of optical pump-probe experiments [1]. The microscopic character of the theoretical model allows to study the impact of distinct scattering processes separately.

In specific, the role of Auger processes is studied. These processes, which are enabled by the linear and gap-less band structure of graphene, modify the carrier density by bridging conduction and valence band. The calculations reveal that Auger scattering gives rise to a significant multiplication of optically excited charge carriers, i.e. multiple charge carriers are generated by the absorption of a single photon [2]. This effect may improve the efficiency of opto-electronic devices, e.g. the sensitivity of graphene-based photodetectors may be increased.

[1] M. Breusing *et al.*, Phys. Rev. B **83**, 153401 (2011); S. Winnerl *et al.*, Phys. Rev. Lett. **107** 237401 (2011) [2] T. Winzer *et al.*, Nano Lett. **10**, 4839 (2010); T. Winzer *et al.*, Phys. Rev. B **85**, 241404(R) (2012)

[Team 3]

First principles investigations on nano materials

Johnny Changeun Kim

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Fundamental understanding about nanostructured materials has led to greater advances in materials science than ever before. Effective computational tools such as density-functional-theory provides viable solutions to resolve the unseen picture beyond the physical limit human effort can reach. In this workshop session, the author present interesting physical properties calculated from various nanostructured materials systems. Coherent thin film, strained thin film, strained bulk phase, amorphous phase, defective structure are examined. Wide range of materials system will be introduced briefly, and the choice of materials include TiN/MgO, IV-VI narrow gap semiconductor, V-VI anisotropic semiconductor, various polymorphs of antimony oxides, and amorphous zirconia. In the last section, the author present some of the progress in understanding thermoelectric property of a materials, and an effort to overcome current limitation caused by frozen band approximation as implemented in common calculation tools.

[Team 3]

Study of semiconducting and metallic 2D compounds

Woosun Jang

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In these days, 2D materials represented by graphene, is strongly highlighted because of its outstanding properties like electrical conductivity, strong strength, good durability , which is far better from preexisting 3D bulk structures. However, there are many limitaions which forbids graphene to applied in industrial area. Therefore, demands for another 2D material which has similarly good properties has popped up.

For the metallic 2D structure, transition metal dichalcogenides (TMDCs), the compound of transition metal and group 6 elements, has various good properties similar to graphene. However, there are not many experiments or calculations of TMDC systems done in order to understand the origin of these properties in various atmospheres. For the semiconducting structure, ultrathin structure of silicon is studied. Silicon has bandgap of 1.1 eV. However, recently, there was a strange observation of silicon bandgap(Prof. HJ Choi), having bigger bandgap behaving like an insulator. It is unusual and not matching with other results, and also its cause is not well discovered yet.

In my research, for metallic structure, I will study 2D TMDCs by using DFT (Density-functional-theory) + vdW which can accurately calculate van der waals correlation in 2D system. For semiconducting structure, by considering different structure models like pandey model, I will discover why this strange big bandgap has observed by carrying out the calculations and analysis of various properties and behaviors.

[Team 2]

Effects of Doping on the Concentrations of Defects at Metal-Oxide Surfaces

Norina A. Richter

Fritz Haber Institute of the Max Planck Society, Berlin, Germany

and

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Doping, either intentional or unintentional, can affect the charge state, the concentration, and the distribution of defects in a material. However, an understanding of the different mechanisms and relative significance of these effects has so far been missing. I will present part of my PhD work, where we consider the charge-carrier conductivity due to doping as a possible thermodynamic factor in the context of defect formation. As a technologically relevant example, surface oxygen vacancies (F centers) in MgO are studied. Defect formation energies are determined using *ab initio* atomistic thermodynamics in combination with hybrid density-functional theory (DFT), with parameters of the exchange-correlation functional optimized according to a condition on DFT ionization energies. Formation energies for neutral defects are validated by coupled-cluster CCSD(T) calculations for embedded clusters. The virtual-crystal approximation [1] is used for a realistic modeling of doping. It is found that at catalytically relevant conditions charge transfer between surface defects and bulk dopants leads to formation of a macroscopically extended space-charge region. The concentration of F_s^{2+} centers at the (100) terrace of p-type MgO can be as high as 1%, while F_s^+ and F_s^0 concentrations are negligible both in p-type and n-type MgO [2]. — [1] L. Veg-

ard, Z. Phys. **5**, 17 (1921); [2] N. A. Richter, S. Sicolo, S. V. Levchenko, J. Sauer, and M. Scheffler, Phys. Rev. Lett. **111**, 045502 (2013).

Note: Subsequent to my presentation, I will give a brief overview on my future research plans concerned with the stability of non-conventional PEM fuel-cell electrodes with platinum single-atom catalysts.

[Team 2]

Magic to stabilize intermediate surface structures of ceria on reduced CeO_2:A first-principles investigation

Collins Lee

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Reducible oxides play an important role in heterogeneous catalysis, because of their ability to store or release oxygen [1] . For ceria, namely CeO_2 in common with other reducible oxides, the in-depth understanding and control of the type, density, and distribution of surface near oxygen vacancies provide a means to influence the electronic structure and to tailor the systems functionality. To date, there is a notable lack of consistency between experimental results on whether oxygen vacancies are more stable at surface or subsurface sites and on whether they attract or repel. However, recently, Gustavo found for a wide range of reducing conditions, the most stable phase is ordered subsurface vacancy structures with all vacancies being third nearest neighbors in the oxygen, showing repelsive interaction [2]. Also, Stetsovych et al. demonstrated ordered reduced phases of ceria in form of thin fims on single crystalline in stead of powder form, by the interfacial reaction between a ceria thin fim and a Ce metal deposit. The thin films include $(\sqrt{7} \times \sqrt{7})$R19.1, (3×3) and cubic Ce_2O_3 (4×4) reconstructions, controlling the amount of Ce deposit [3]. In this work we consider different surface reconstruction structures including recently proposed intermediate bulk termination models as compared to previous reported stable structures with repulsive oxygen vacancies. Especially we construct slab models from well known (2×2) to cubic Ce_2O_3 (4×4) to prove recent experimental results in theoretical perspective,

depending oxygen stoichmetry changes. Also we investigate the influence of lattice strain and monolayer depth on CeO_2 cubic of reconstruction surfaces to surface stability. Via applying different lattice constants with variation from -7% to +2% with repect to standard CeO_2 bulk truncated one (3.88 Å), we found strong correlation between strained structure and its properties. And we produce firm computational evidence that different depth profiles of surface and subsurface z-direction geometery show different structural stability.

[1] *Science* **301** 935 (2003)

[2] *Phys. Rev. Lett.* **110** 246101 (2013)

[3] *J. Phys. Chem. C* **118** 357 (2014)

[Team 2]

TiN, Pt, MTG and Me

Rachael Tak

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Platinum is one of the most broadly used catalyst for many chemical reactions (e.g. oxygen reduction reaction). Although it's great reactivity, platinum catalysis has not met enthusiastic reception from industry due to its high price. Pt/C catalyst is widly used to come up this problem, but still considered as an imperfect solution because of its bad stability. Recently, Transition metal nitrides (TMNs) are studied as promising support material for next generation platinum catalyst. According to stream of catalyst study, MTG has been studied about titanium nitride and titanium nitride supported platinum catalyst. In this study, we put platinum layers on TiN (100) surface, as an effort for reduce platinum loading, and determined own properties. We calculated its lowest energy structure, bond length and electronic structure by density-functional theory (DFT). Moreover, trend study of different d-transition metals (Pt, Ir, Ni, pd and Au) will be reported to understand d-transition metal's electronic nature and compare with Pt, which is most famous electrocatalyst. These d-transition metals are also put on TiN subsrate and most stable structure will be presented in this study. Vienna Ab initio simulation package (VASP) is used for this study.

[Team 1]

The introduction to Su-Hyun's research themes

Su-Hyun Yoo

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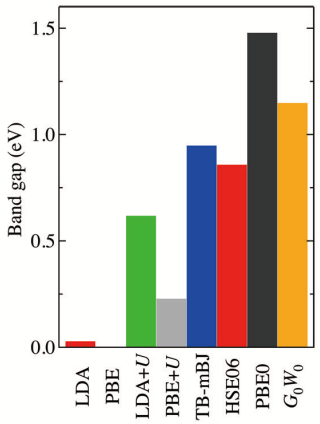
The each of my research topics will be briefly introduced in this talk. The main research themes of mine are basically broken into 2 parts, surface science and bulk electronics.

First of all, my internship topic in final year of undergraduate, *electronic structure and band alignment of* Zn_3N_2, will be presented. The band gap energy of Zn_3N_2 and the studied feature of each *xc*-functionals, from LDA to quasi-particle perturbation theory G_0W_0, would be mainly discussed.

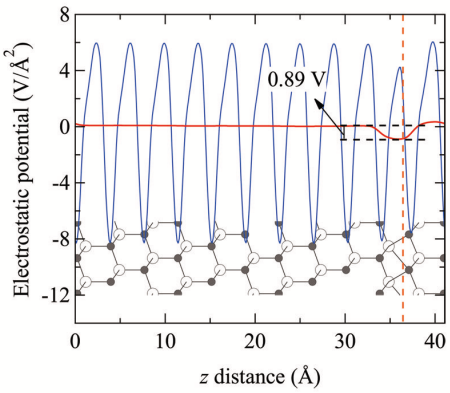
Second, the study of tacking faults (SF) in CdTe which I have investigated in UK for 2-month, will be presented. It is well known that the annealing treatment toward CdTe photovoltaic devices is essential in order to achieve high efficiency. We thought the SF plays a important role for this mechanism. The specific SF which strongly affects on the electronic properties of CdTe is introduced, and as well as the effect of twin boundaries is also discussed at the same time.

Lastly, the master thesis topic, nanomorphology of Pd particles under Br and K environment, will be presented. The morphological evolution of Pd nanoparticles predicted based on Gibbs-Wulff theorem will be mainly talked, and as well as studied *ab initio* thermodynamics will be explored. Simultaneously, the plan for this further study is introduced.

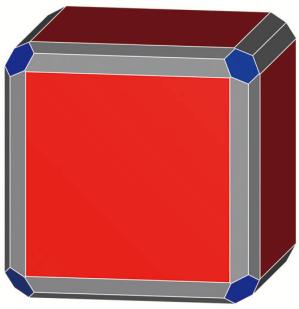
Zn_3N_2



CdTe



Br & K / Pd



[Team 1]

What Michael have been studied

Ji-Hwan, Michael Lee

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In this MTG-MICE, I will summarize my research results of three years. For last three years, my research topics have been composed of two parts, renewable energy and thermodynamics of interface by using density-functional theory. Because of the limitation of natural fuels, my first keyword "Renewable energy" is the biggest topic for me in order to contribute for the whole research society. Also various atomistic understandings of interfaces in heterogeneous catalyst or grain boundaries are also scientifically important issues.

By these reasons, I had one and half years of experience in experimental group, which synthesizes Solid Oxide Fuel Cell (SOFC) in low-temperature using GDS, YSZ and NiO by sintering and Pechini process, and analyzes the operating SOFC devices electrochemically .

As a member of Material Theory Group, my research experience could be seperated by 3 parts: internship, collarboration and my own projects. As an intern, the anisotropic mechanical properties of condensed materials, such as TiN, Diamond etc, has been studied. After then, my TiN/MgO project started with other two collarbolation works; Brodium project of Daniel and TinCubell project of Emmanuel. The aim of TiN/MgO project is to understand the thermodynamic stability of the system and electronic interaction in the interface.

In conclusion, I hope my research is well heading to the thermodynamics of interface system and be able to observe in renewable energy society although these topics are little bit spread out.

[Team 1]

DFT study of surface alloy of Sn/Cu(100)

Jongmin Yun

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To date, the explicit atomic geometry of high surface coverage structure of Sn/Cu(001)is still strongly debated in the same context. Particularly, Layer deposition of Sn on Cu(001) can give rise to a rich variety of surface reconstructions in the sub-monolayer surface coverage range of Sn.[1][2][3][4] Thus, using density-functional theory coupled with the ab initio atomistic thermodynamics (AIAT) approach [5], we attempted to map out the *ab initio* surface phase diagram of the Sn/Cu(001) system. We plotted the graph about Gibbs free energy change versus chemical potential energy change of Tin so that we can theoretically derive the structures of surfaces and phase diagram based on the calculation results of each model's binding energy through AIAT. We hope this result to provide insight into the rich surface chemistry of this near-surface alloy system. In particular, I will present the binding energies, electronic structure (i.e. workfunction), and the atomic geometries of various interesting surface reconstructions of Sn on Cu(001) as a function of Sn surface coverage. Through this work, we aim to reconcile the different experimental findings reported in past literature, and provide a more congruent picture of the Sn/Cu(001) system. And comparison with experimental STM image will be done for more detailed contemplation. And by using work-function values which belong to various surfaces of bulk phases of Sn, possibility of work-function tuning will be referred. Furthermore, the un-converged surface energy of Sn Beta (001) will be suggested as a side talk. This will be debated with figure of density of

states and electro-potential plots.

[1] *Surf. Sci.* **601**, 5170 (2007) [2] *Surf. Sci.* **549**, 24 (2004); [3] *Surf. Sci.* **605**, 1000 (2011); [4] *Surf. Sci.* **603**, 341 (2009) [5] *Catal. Today.* **105**, 17 (2005)

[Team 1]

Wetting and the effect

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Wetting phenomena have been observed everywhere around us in nature where liquid material is on a rigid solid material. Special phenomena in nature about the wetting have arrested researchers attention for example, superhydrophobic property of the lotus, so called lotus effect. Wetting has deeply studied for the applications using extra phobic and philic property between liquid and solid material for decades due to the utility of it. Here, this presentation will start with the mechanism of the wetting and also show the well known basic wetting models. The effects and the examples will be also presented for the comprehension of the wetting.

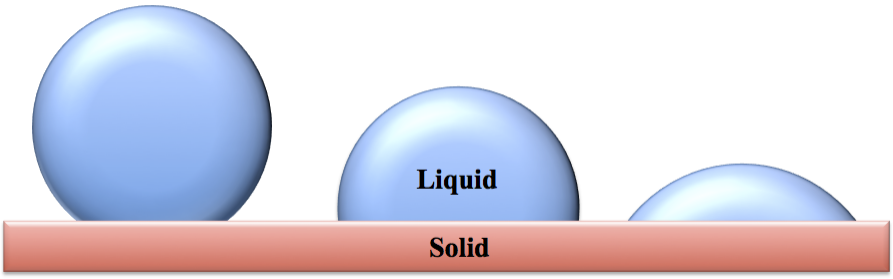

Figure 1: Wetting phenomena with various wettability.