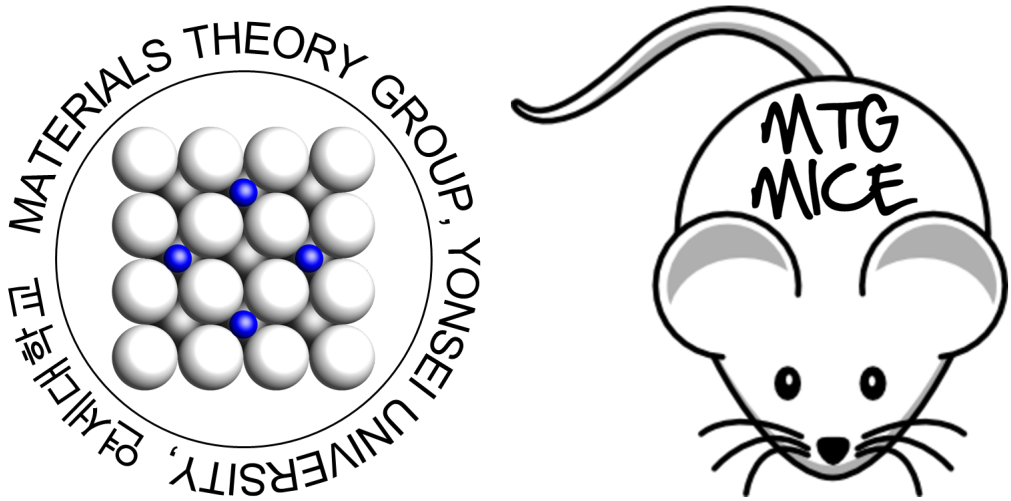
Workshop in 2017

The 10th Materials Information, Characterization, and Exploration (MICE-10)

B127, Engineering Building B, Yonsei University, Seoul, Korea

February 24th Friday 2017



Organized by Materials Theory Group, Yonsei University, Korea

MICE-10 Schedule

Time	Title	Speaker
11:00 ~ 11:10	MICE-10 Opening Announcement	Aloysius Soon
11:10 ~ 11:40	Influence of Rb/Cs cation-exchange on inorganic Sn halide perovskites: From chemical structure to physical properties	Young-Kwang Jung
11:40 ~ 12:10	Engineering the Colossal Magnetoresistance by Orbital Modulator Thin Film	Jongmin Yun
12:10 ~ 13:10	**Lunch**	
13:10 ~ 13:40	The surface energy study of hexagonal closed pack metals	Ji-Hwan Lee
13:40 ~ 14:10	Eventual Chemical Transformation of Metals and Chalcogens into Metal Chalcogenide M_2X_3 Nanoplates through Surface Nucleation-Coming Off-Reorganization Mechanism	Jiwoo Lee
14:10 ~ 14:40	Nanoporous transition metal oxides for water desalination applications	Woosun Jang
14:40 ~ 15:10	**Coffee break**	
15:10 ~ 15:25	How can we study on nanotoxicity of nanomaterials by ab initio methods?	Ungcheon Kim
15:25 ~ 15:40	Theoretical study about the polymorphism for over valence charge state materials of TaO_3	Yunjae Lee
15:40 ~ 16:10	Polymorphic Phases of Hexagonal Tungsten Trioxide: Relative Stabilities and Electronic Structures	Yong-Hyuk Lee
16:10 ~ 16:40	Comprehensive Studies on Copper Surface Oxide: Surface Science Approaches	Taehun Lee

Content of Abstracts

[11:10 - 11:40]

Influence of Rb/Cs cation-exchange on inorganic Sn halide perovskites: From chemical structure to physical properties

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$CsSnI_3$ is a potential inorganic lead-free inorganic perovskite for solar energy applications due to its non-toxicity and attractive optoelectronic properties. [1-3] In spite of these advantages, photovoltaic cells using $CsSnI_3$ have not been successful to date, in part due to low stability. We demonstrate how gradual substitution of Rb for Cs influences the structural, thermodynamic, and electronic properties on the basis of first-principles density-functional theory calculations. By examining the effect of Rb:Cs ratio, we reveal a correlation between octahedral distortion and band gap including spin-orbit coupling. We further highlight the cation-induced variation of the ionisation potential (work function) and the importance of surface termination for tin-based halide perovskites for engineering high-performance solar cells.

[1] I. Chung, J.-H. Song, J. Im, J. Androulakis, C. D. Malliakas, H. Li, A. J. Freeman, J. T. Kenney, M. G. Kanatzidis, *J. Am. Chem. Soc.* **134**, 2224 (2012)

[2] Z. Chen, C. Yu, K. Shum, J. J. Wang, W. Pfenninger, N. Vockic, J. Midgley, J. T. Kenney, *J. Lumin.* **132**, 345 (2012)

[3] K. Shum, Z. Chen, J. Qureshi, C. Yu, J. J. Wang, W. Pfenninger, N. Vockic, J. Midgley, J. T. Kenney, *Appl. Phys. Lett.* **96**, 221903 (2010)

[11:40 - 12:10]

Engineering the Colossal Magnetoresistance by Orbital Modulator Thin Film

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Controlling the magnetism by magnetic field, called as colossal magnetoresistance (CMR) is important phenomenon which can be applied on multifunctional devices such as all oxide spin FETs, magnetic tunnel junctions, and non volatile MRAM as multiferroic memory [1-2]. One of the focused material with CMR is $LaMnO_3$ (LMO) because of several results. Not only doping hole with Ca into LMO [3], but also deformation by inducing pressure modulate the AFM to FM conversion is found in LMO, which called "bad metal" behavior [4]. Based on these phenomena, orbital modulator nanopatterning has been suggested. However, the detailed mechanism of interplay between structural deformation (i.e. Jahn-Teller distortion) and chemical modulation is not reported. Therefore, we suggest to evaluate the structure and magnetic properties of orbital modulating metals on LMO in order to examine the possibility of designing the nano-patterned CMR device and understand this phenonmenon.

[1] A.-M Haghiri-Gosnet and J.-P Renard *et al. J. Phys. D: Appl. Phys.* **36**, R127 (2015)

[2] H. Guo *et al. Adv. Mater. Interfaces* **3**, 1500753 (2016)

[3] M. Fäth *et al. Science* **285**, 1540 (1999)

[4] M. Baldini *et al. P. Natl. Acad. Sci. USA* **112**, 10869 (2015)

[13:10 - 13:40]

The surface energy study of hexagonal closed pack metals

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A fast and efficient way to calculate accurate surface energy for body-centered cubic and face-centered cubic metas is reported in our previous works. [1] However, the more complex system such as hexagonal-closed pack (*hcp*) metal which include identical two atom in unit cell are not fully developed. In this study, we evaluate various methodology reported previously and improve the broken bond model based on density-functional theory calculation.

[1] Su-Hyun Yoo *et al.*, *Phys. Rev. B* **93**, 035434 (2016)

[13:40 - 14:10]

Eventual Chemical Transformation of Metals and Chalcogens into Metal Chalcogenide (M_2X_3) Nanoplates through Surface Nucleation-Coming Off-Reorganization Mechanism

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Many studies have reported the synthesis of 2D nanoplates and nanosheets of the layer-structured metal chalcogenides. [1] In multicomponent compounds, the elemental concentrations and struntures keep changing during the reaction and this non-stoichiometric reactions cause different shapes of the metal chalcogenides. [2] However, the mechanism involved and whether such non-stoichiometric reactions eventually produce 2D nanoplates has not been studied yet. Here we investigates a two-step chemical reaction as an extreme non-stoichiometric nucleation and growth. It reveals that the layer-structured metal chalcogenides (M_2X_3, M=Sb/ Bi, X=Se/ Te) can be obtained by transforming premade pure chalcogen (Se, Te) thick nanorods or metal microparticles (Bi). By coupling our first-principles calculations with a shape-prediction thermodynamic model, we have examined the shape/aspect ratio of the M_2X_3 nanocrystals under different experimental growth conditions. The tendency of anisotropic growth to form the 2D shapes during the transformations are discussed on the basis of experimental results and theoretical calculations.

[1] G. Zhang, W. Wang, X. Lu, and X. Li, *Cryst. Growth Des.* **9**, 145 (2009)

[2] Y. Min, J. Kwak, A. Soon, and U. Jeong, *Acc. Chem. Res.* **47**, 2887 (2014)

[14:10 - 14:40]

Nanoporous transition metal oxides for water desalination applications

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Many traditional approaches of water desalination already faced a challenge on providing potable water to meet the demands of the globe's population. As an alternative mean, water purification system using two-dimensional (2D) nanoporous materials as a membrane, is considered to be the potential candidate to replace conventional methods, due to the large surface area and high mechanical strength of 2D materials. However, owing to the difficulties in synthesizing large-scaled and single-layered crystals of 2D materials, only a few of 2D materials have been exploited for water desalination applications, and are still in the infancy stage. Here, we suggest the porous transition metal oxides for water desalination applications, which have a great advantage over other 2D materials, originated from their intrinsic atomic channels.

[1] S. Dervin, D. D. Dionysiou, and S. C. Pillai, *Nanoscale* **8**, 15115 (2016)

[2] J. Liu, G. Shi, and H. Fang, *Nanotechnology* **28**, 084004 (2017)

[3] Y. Lee, T. Lee, W. Jang, and A. Soon, *Chem. Mater.* **28**, 4528 (2016)

[4] J. Yun, W. Jang, T. Lee, Y. Lee, and A. Soon, *Phys. Rev. Applied., accepted*

[15:10 - 15:25]

How can we study on nanotoxicity of nanomaterials by ab initio methods?

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Nanotechnology has developed at a over the past decade, with applications in many sectors. [1] Accordingly, the matter of safety and toxicity of nanomaterials has become an issue of interest to the public. [1] In an effort to assess these hazards, the field of nanotoxicology (studying toxicity of nanomaterials) has been addressed. [1] Nanotoxicity occurring mechanisms are mainly oxidative stress via overproduction of reactive oxygen species(ROS). [1] It can leads to DNA damage, cytotoxicity etc. [1] Among the ROS inducing nanomaterials, Metal oxides are the most widely used types of engineered nanomaterials. [1] Nano-metal oxides with redox characteristic properties can enhance the formation of ROS, serving as catalysts in ROS production. Understanding these mechanisms of nanomaterial-induced toxicity is the first defense for hazard prevention. [1] For this understanding, I will consider CuO. CuO NPs are being used in various applications which it turned out that nano-CuO exhibits the highest cytotoxicity and genotoxicity. [2] Till now, there is no specific study to provide the first stage towards attempting to understand ROS formation. So I will study this by first-principles methods to see which site H_2O_2 on the nanometal cluster or slab is adsorbed at, what the detaild path is that this each reaction takes etc.

[1] Peter P. Fu *et al.*, *Journal of food and drug analysis*, **22**, 64 (2014)

[2] HL Karlsson *et al.*, *Chem. Res. Toxicol*, **21**, 1726 (2008)

[15:25 - 15:40]

Theoretical study about the polymorphism for over valence charge state materials of TaO_3

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Transition metal oxide, for example, TiO_2, Cu_2O, WO_3, MoO_3, is the multifunctional materials such as in electronics, optics, catalysis etc. In order to their diversity of polymorphism, transition metal oxide is actively investigated for the various properties following with various oxidation state and polymorphism. Tantalum oxide is also the key materials for electric device [1] and usually +4 and +5 valence charge state of Ta is well known for the tantalum oxide. But experimentally, 2D nanosheet of TaO_3, which is 6+ valence charge state of Ta, is synthesized and has the good properties for lithium ion battery [2]. More over, 3-dimentional ReO_3 structure of TaO_3 is studied theoretically and the structure is well stabilized thermodynamically and elastically [3]. These results show the possibility of over valence state material. Previously, there are many studies about the polymorphism of WO_3 and MoO_3, which is also 6+ state of W and Mo. So with these structures, we investigate the polymorphism of TaO_3 and the various properties with each structure. Our results will be the fundamental study for expending the field of mateials with over valence charge state.

[1] C. Chaneliere *et. al.*, *Mat. Sci. Eng.*, **22**, 269 (1998)

[2] X. Xu *et. al.*, *Energy Environ. Sci.*, **4**, 35 (2011)

[3] C. Ravi *et. al.*, *Comput. Mat. Sci.*, **90**, 177 (2014)

[15:40 - 16:10]

Polymorphic Phases of Hexagonal Tungsten Trioxide: Relative Stabilities and Electronic Structures

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In line with developments in synthesis techniques, metastable phases of heavy metal oxides have been in the center of interest due to their unique chemical and physical properties and possibilities as promising devices. [1] In these metastable phases, to figure out the precise atomic structures is highly important because small distortions or structural modifications can cause significant changes in their electronic structures. [2, 3] However, there remain scientific challenges to analyze precise atomic structures with experiments. As an example, there have been controversies of bulk hexagonal tungsten trioxide (h-WO_3) crystalizing in different crystal symmetries–$P6/mmm$, $P6_3/mcm$ and $P6_3cm$, and depending on the structures, calculated electronic band gap can be open $\sim 1\,\mathrm{eV}$. [3-5] In this work, we present a first-principles density-functional theory to investigate stabilities and corresponding electronic structures of bulk h-WO_3 polymorphes.

[1] B. Miao *et al.*, *Mater. Lett.* **147**, 12 (2015)

[2] Y. Ping, Y. Li, F. Gygi, and G. Galli, *Chem. Mater.* **24**, 4252 (2012)

[3] P. Krüger, I. Koutiri, and S. Bourgeois, *Phys. Rev. B* **86**, 224102 (2012)

[4] B. Gerand *et al.*, *J. Solid State Chem.* **29**, 429 (1979)

[5] D. Saha *et al.*, *Angew. Chem. Int. Ed.* **53**, 3667 (2014)

[16:10 - 16:40]

Comprehensive Studies on Copper Surface Oxide: Surface Science Approaches

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The embryonic ultrathin oxide layers so called "surface oxide" are early stages of metal oxidation, possessing distinct structural and electronic properties, as compared to their parent bulk metals and oxides. [1] As a representative example of complex surface oxide systems, copper surface oxides are promising candidates for modern industrial catalysts due to their high chemical activities for versatile reactions. [2] Relying on the oxygen content and preparation temperature, different copper surface oxide structures have been observed and there have been several theoretical works to understand their physical and chemical properties, matching with relevant experiments. [3-4] Here, our investigations reveal accurate relative phase stabilities of copper surface oxide layers on copper (111) substrate as a comprehensive study and also bridge theoretical examinations with experimental observations by conducting theoretical spectroscopic and topological analysis.

[1] H.-J. Freund and G. Pacchioni, *Chem. Soc. Rev.* **37**, 2224 (2008)

[2] C. Gattinoni and A. Michaelides, *Surf. Sci. Rep.* **70**, 424 (2015)

[3] C. P. León, C. Sürgers and H. V. Löhneysen, *Phys. Rev. B* **85**, 035434 (2012)

[4] A. Soon, M. Todorova, B. Delley and C. Stampfl, *Phys. Rev. B* **73**, 165424 (2006)