THIS
THEORY OF HETERO-INTERFACES AND SURFACES

6th July 2018 (Friday)
Engineering Building IV (#124), Level 4, Room D407
Yonsei University, Seoul, S. Korea

Time	Program
09:50 – 10:00	Lecture 0 Welcome and introduction **Prof. Aloysius Soon** (*Yonsei University, S. Korea*)
10:00 – 10:45	Invited Talk Non-oxidizing grain-free wafer-scale copper thin film and its applications **Prof. Se-Young Jeong** (*Pusan National University, S. Korea*)
10:45 – 11:30	Invited Tutorial STM simulations based on DFT: The 3D-WKB-STM and BSKAN codes **Dr. Krisztián Palotás** (*Hungarian Academy of Sciences, Hungary*)
11:30 – 12:15	Invited Talk STM studies on the 2D layered materials **Prof. Jungdae Kim** (*University of Ulsan, S. Korea*)
12:15 – 13:30	Lunch time
13:30 – 14:15	Invited Tutorial Imaging mechanism of SPM using flexible tip apexes and simulations of flexible tip apex employing fm-AFM images of (2D) molecules adsorbed on (metal) surfaces **Dr. Ondřej Krejčí** (*Aalto University, Finland*)
14:15 – 14:35	Contributed Talk Ionic conductivity and activation energy for oxygen ion transport in superlattice-ScSC/YSZ and SDC/YSZ **Dr. Mehmet Emin Kılıç** (*Yonsei University, S. Korea*)
14:35 – 14:55	Contributed Talk RGB colors of copper thin film by the accurate control of oxidation **Dr. Su-Jae Kim** (*Pusan National University, S. Korea*)
14:55 – 15:15	Coffee break
15:15 – 15:35	Contributed Talk Atomistic study on the surface structures of Cu_2O (111) **Ms. Thi Ly Trinh** (*University of Ulsan, S. Korea*)
15:35 – 15:55	Contributed Talk The fundamental understanding of hexagonal tungsten trioxide (h-WO_3) from bulk to the surface with its potential applications **Mr. Taehun Lee** (*Yonsei University, S. Korea*)
15:55 – 16:30	Free discussion (optional)

STM simulations based on DFT: The 3D-WKB-STM and BSKAN codes

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Scanning tunneling microscopy/spectroscopy (STM/STS) is a very useful tool for wide areas of nanoscience and nanotechnology to study local physical/chemical properties of material surfaces. In the talk a brief introduction to different levels of electron tunneling theories is given, followed by a presentation of two simulation tools, the 3D-WKB-STM [1] and BSKAN [2,3] codes that allow the high-resolution STM/STS calculations of various material surfaces based on ab initio density functional theory (DFT) electronic structure data. Such STM simulation tools are inevitable for the proper interpretations of experimental STM images. A few examples are highlighted, where the STM tip plays a crucial role [4,5,6,7,8], and a prediction of spin-polarized STM contrasts of a diversity of topologically protected magnetic skyrmions is provided [9,10]. Finally, a practical guidance for the usage of the presented STM simulation tools is given.

References

1. K. Palotás, G. Mándi, W. A. Hofer, *Front. Phys.* 9, 711 (2014).
2. W. A. Hofer, *Prog. Surf. Sci.* 71, 147 (2003).
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5. G. Mándi, N. Nagy, K. Palotás, *J. Phys. Condens. Matter* 25, 445009 (2013).
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10. K. Palotás, *arXiv:1804.09096* (2018).

Imaging mechanism of SPM using flexible tip apexes and simulations of flexible tip apex employing fm-AFM images of (2D) molecules adsorbed on (metal) surfaces.

Abstract: In this talk I will briefly introduce imaging mechanism of scanning probe microscopy (SPM) techniques using flexible tip apexes, like CO or Xe-tip [1-3]. I will focus mainly on frequency-modulation atomic force microscopy (fm-AFM), but I will also briefly mention scanning tunneling microscopy (STM) [4,5] and inelastic electron tunneling spectroscopy (IETS) imaging [6,7]. Are the bright lines in fm-AFM images really bonds [1,2,8]?
After that I will focus on probe particle code [2,3,9], which can be used for simulations of the fm-AFM obtained with flexible tip apexes. I will run couple of examples of simple simulations, show some results of more sophisticated calculations as well as I will present most recent development of the code that uses graphic cards and is able to visualize simulated *df*-images in couple of seconds on a standard work station or laptop.
If times allows, then in the end I would like to introduce also work of other theoreticians from the field: Work of N. Moll calculating Pauli repulsion from total-electron density [10]; Fitting complex electrostatics of the CO tip [11,12] and atom-pair interaction to DFT (and experimental) data [11]; Obtaining electrostatic field around the molecule from experimental measurements [12]; And using model for both atoms of CO-tip [13].

References:
[1] Gross *et al.*, Sci. 325, 1110 (2009)
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