2016

Dr. Poe Lecture Hall
Institute of Atomic and Molecular Sciences
Academia Sinica, Taipei, Taiwan

November 13 ~ 16

& Asia-Pacific Symposium on Solid Surfaces
Cross-Strait Symposium on Solid Surfaces

PROGRAM

"Asia-Pacific Symposium on Solid Surfaces & Cross-Strait Symposium on Solid Surfaces" Program

	11/13 (Sunday)	11/14 (Monday)	11/15 (Tuesday)	11/16 (Wednesday)
08:30—09:00		**Registeations**		
09:00—09:20		**Welcome Opening Speeches**	Minn-Tsong Lin	Ying-Hao Chu
09:20—09:40		Alexander A. Saranin	Sergei. V. Zaitsev-Zotov	Deng-Sung Lin
09:40—10:00		Iwao Matsuda	Ya-Ping Chiu	Ho Ki Lyeo
10:00—10:20		Dimitrii. V. Gruznev	Wei-Bin Su	Woei-Wu Pai
10:20—10:40		Satoru Ichinokura	Yanjun Li	**Break (10:20 - 10:50)**
10:50—11:10		**Break (10:40 - 11:10)**	**Break (10:40 - 11:10)**	Meng-Fan Luo
11:10—11:30		Xi Chen	Shu-Jung Tang	Chuanshan Tian
11:30—11:50		Nikita Denisov	Sukmin Jeong	**Closing Remarks and Farewell (11:30 - 11:40)**
11:50—12:10		Tien-Ming Chuang	Joung Real Ahn	**Lunch (12:00 - 13:30)**
12:10—14:00		**Lunch**	**Lunch**	
14:00—14:20		Yasuhiro Sugawara	Mei-Yin Chou	**Ride to Visit National Synchrotron Radiation Research Center or National Palace Museum**
14:20—14:40		Geunseop Lee	Han Woong Yeom	
14:40—15:00		Aleksei Mikhaliuk	Shiwei Wu	
15:00—15:20		**Break (15:00 - 15:30)**	Feng Miao	
15:30—15:50		Shangir Gwo	**Break (15:20 - 15:50)**	
15:50—16:10		Andrey V. Zotov	Se Jong Kahng	
16:10—16:30		Kazushi MiKi	S.V. Eremeev	
16:30—16:50	**Reception** (In IAMS)	**Poster Presentation (16:30 - 18:00)**	Christopher J. Butler	
16:50—17:10			Andrey V. Matetskiy	
17:20—18:00			**Ride to the Restaurant**	
18:00—		**Buffet Dinner**	**Conference Banquet**	

Day / Time	11/14 (Monday)	
08:30~09:00	**Registration**	
09:00~09:20	**Welcome Opening Speeches**	
Session Chair : Shuji Hasegawa		
09:20~09:40	Alexander A. Saranin	Atomic Structure and Electronic Properties of the Si(111)-**√3×√3**-(Tl, A) (A=Group IV, V, VI) Compounds
09:40~10:00	Iwao Matsuda	Electronic Structures of the Novel Monatomic Layers Topology of the Famous Multilayers
10:00~10:20	Dimitrii. V. Gruznev	Long-range-ordered 2D Tl-Pb Compounds on Si(111) and Ge(111)
10:20~10:40	Satoru Ichinokura	Superconducting Properties of Tl Double Atomic Layer on Si(111)
10:40~11:10	**Break**	
Session Chair : Alexander A. Saranin		
11:10~11:30	Xi Chen	Superconductivity and Anomalous Enhancement Induced by Impurities in Two-dimensional Non-centrosymmetric Monolayer $NbSe_2$
11:30~11:50	Nikita Denisov	MBE Grows of Superconducting β-$PdBi_2$ Films
11:50~12:10	Tien-Ming Chuang	Superconducting Topological Surface States in Non-centrosymmetric Bulk Superconductor $PbTaSe_2$
12:10~14:00	**Lunch**	
Session Chair : Chia-Seng Chang		
14:00~14:20	Yasuhiro Sugawara	Atomic-resolution Simultaneous Imaging of Topography, Surface Potential and Dipole Moment on TiO_2(110) Surface
14:20~14:40	Geunseop Lee	How the Phase Transition of Si(111)In-4x1 Proceeds and Is Affected by Various Impurities
14:40~15:00	Aleksei Mikhaliuk	Atomic Structure of Thallium Double Atomic Layer on Si(111)-**6√3×6√3**
15:00~15:30	**Break**	
Session Chair : Xi Chen		
15:30~15:50	Shangir Gwo	Metal–Oxide–Semiconductor Plasmonic Nanorod Lasers
15:50~16:10	Andrey V. Zotov	2D Adsorbate Compounds on Silicon: Experiment versus Theory

16:10~16:30	Kazushi MiKi	Monolayer-Digital Magnetic Alloy (DMA) Formed at the Interface of a-Ge/Mn chain/Si(001)
16:30~18:00	**Poster Presentation**	
18:00~	**Buffet Dinner**	

Day / **Time**	**11/15 (Tuesday)**	
08:30~09:00	**Registration**	
Session Chair : Han Woong Yeom		
09:00~09:20	Minn-Tsong Lin	Scanning Tunneling Spectromicroscopy Study on Spintronic Emergent Materials
09:20~09:40	Sergei. V. Zaitsev-Zotov	Effect of Chemical Potential Shift on Energy Gap Detection by Scanning Tunneling Spectroscopy
09:40~10:00	Ya-Ping Chiu	Influence of Ferroelectric Polarization on Superconducting Behaviors at $BiFeO_3/YBa_2Cu_3O_{7-\delta}$ Heterointerface
10:00~10:20	Wei-Bin Su	Sharpness-Induced Energy Shifts of Quantum Well States and Its Applications
10:20~10:40	Yanjun Li	The Investigation of Local Dipole Moment on TiO_2(110) Surface by Electrostatic Force Microscopy
10:40~11:10	**Break**	
Session Chair : Chin-Ming Wei		
11:10~11:30	Shu-Jung Tang	Control of the Dipole Layer of Polar Organic Molecules on Metal Surfaces
11:30~11:50	Sukmin Jeong	Adsorption Chemistry of Aromatic Molecules on Si(5 5 12)
11:50~12:10	Joung Real Ahn	Designed Three Dimensional Graphene Architecture
12:10~14:00	**Lunch**	
Session Chair : Yuh-Lin Wang		
14:00~14:20	Mei-Yin Chou	Interplay of Charge and Lattice Distortion in Few Layers of Transition Metal Dichalcogenides
14:20~14:40	Han Woong Yeom	Creating Heterointerfaces with Textured Electronic States on Correlated Transition Metal Dichalcogenides

14:40~15:00	Shiwei Wu	Folding, Stacking and Stitching of Transition Metal Dichalcogenide Monolayers
15:00~15:20	Feng Miao	Electronic Transport and Device Applications of 2D Materials
15:20~15:50	**Break**	
Session Chair : Andrey V. Zotov		
15:50~16:10	Se Jong Kahng	Reversible Manipulations and Detections of Spin-Trans-Effect through Kondo Resonance
16:10~16:30	S.V. Eremeev	Rashba and Dirac States in BiTeX (X = Cl, Br, I) Compounds
16:30~16:50	Christopher J. Butler	Atomically Resolved Surface Characterization of the 3-D Dirac Semimetal Cd_3As_2
16:50~17:10	Andrey V. Matetskiy	Dirac Surface States in the Heterostructures of Topological and Trivial Magnetic/Non-magnetic Insulators
17:20~18:00	**Ride to the Restaurant**	
18:00~	**Conference Banquet**	

Day / Time	11/16 (Wednesday)	
08:30~09:00	**Registration**	
Session Chair : Ya-Ping Chiu		
09:00~09:20	Ying-Hao Chu	A Metal-Insulator Transition of the Buried MnO_2 Monolayer in Complex Oxide Heterostructure
09:20~09:40	Deng-Sung Lin	Growth of Ge and Si on the Monolayer Silicene on Ag(111)
09:40~10:00	Ho Ki Lyeo	Thermoelectric Imaging of Structural Disorder in Epitaxial Graphene with Atomic Resolution
10:00~10:20	Woei-Wu Pai	Dual-Phase Single-Layer Germanene on Ag(111)
10:20~10:50	**Break**	
Session Chair : Yuh-Lin Wang		
10:50~11:10	Meng-Fan Luo	Dependence on Size of Supported Rh Nanoclusters in the Decomposition of Methanol
11:10~11:30	Chuanshan Tian	Unveiling Microscopic Structures of Charged Water Interfaces by Surface-Specific Vibrational Spectroscopy
11:30~11:40	Yuh-Lin Wang	Closing Remarks and Farewell
12:00~13:30	**Lunch**	
13:30 ~	**Ride to Visit National Synchrotron Radiation Research Center (國家同步輻射研究中心) or National Palace Museum (國立故宮博物院)**	

Atomic Structure and Electronic Properties of the Si(111)√3×√3-(Tl, A) (A = Group IV, V, VI) Compounds

Saranin AA,[1,2,*] Matetskiy AV,[1] Kibirev IA,[1,2] Gruznev DV,[1] Bondarenko LV,[1] Tupchaya AY,[1] Wei CM,[3] Hsing CR,[3] Mihalyuk AN[1,2], Zotov AV,[1,2,4]

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The Rashba spin splitting [1] in the two-dimensional electron gas systems on semiconductors is considered to be the key concept for many promising spintronics applications. Recently we found a number of the dense two-dimensional one-atom layer reconstructions on Si(111) surface with spin-split metallic bands [2]. One of these reconstructions made of one monolayer of Tl and one-third monolayer of Pb with √3×√3 periodicity was found to exhibit a giant Rashba-type spin splitting of metallic surface-state bands together with two-dimensional superconducting properties [3]. Our investigations revealed that the same type of the reconstruction with the same √3×√3 periodicity, composition and structure can be realized not only for Tl and Pb (Group IV element) but also for Tl and Group V (Bi, Sb) and Group VI (Se, Te) elements. Our results indicate that all of the two-dimensional compounds demonstrate spin split bands while the metallic properties changes dramatically. Compound formed by Tl and Group IV element is metallic with two metallic bands, compounds formed by Tl and Group V (Bi, Sb) elements are also metallic with only one metallic band while compounds formed by Tl and Group VI (Se, Te) elements are semiconducting.

The work was supported by the Russian Science Foundation (Grant 14-12-00479).

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■ Invited talk □ Poster

[1] Y. Bychkov and E. Rashba, JETP Letters **39**, 78 (1984).
[2] D.V. Gruznev et al., Scientific Reports **4**, 4742 (2014).
[3] A.V. Matetskiy et al. Phys. Rev. Lett. **115**, 147003 (2015)

Electronic Structures of the Novel Monatomic Layers Topolgy of the Famous Multilayers

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Rapid progress in the miniaturization of microelectronics devices now forces signal currents to flow near the surface/interface region in crystals, and ultimately, with continued miniaturization, will force the current through only atomic layers. For technical innovations, it has been highly called for to synthesize novel atomic layers and to investigate their functionalities. In this poster, two of our recent photoemission researches are presented. One is electronic states in the novel monolayer boron (B) on Ag(111) and the other is topological edge-states of the famous bismuth (Bi) films on Ge(111).

1・A monolayer boron (B) on Ag(111)

Boron, the fifth element in the periodic table, has been known to be the lightest element substance that forms interatomic covalent bonds. Recently, the discovery of graphene has triggered great interests in the search for elemental monolayer materials and theoretical investigations on the related materials have spurred experimental findings of silicene, germanene and phosphorene. Likewise, monolayer boron has also been explored theoretically and, intriguingly, it has been predicted to be metallic which sharply contrasts the semiconducting nature of the bulk allotropes. Here, we report the results of band mapping by angle-resolved photoemission spectroscopy (ARPES) with a He source, which directly reveal metallic bands in the top boron layer in this system. The photoemission Fermi surface includes one electron pocket centered at the S point and a pair of electron pockets near the X point in the two-dimensional Brillouin zone (2D BZ). The band dispersion curves are in agreement with those calculated by the first-principles calculations on the $_{12}$-sheet structure model. Finding of the metallic bands of monolayer boron is expected to promote further investigations of novel properties such as the superconductivity predicted theoretically in the present $_{12}$-sheet structure model. Moreover, a selective nitridation of the boron monolayer is expected to synthesize insulating boron nitrides that forms insulator-metal junction in the same single layer, enabling the development of all-boron nano-devices.

2・Topological edge-states of bismuth (Bi) films on Ge(111)

Semimetal Bi has recently attracted much attention due to its spin-polarized metallic surface states, which originate from its giant spin-orbit coupling. It makes Bi one of the most central element in designing topological materials such as $Bi_{1-x}Sb_x$, Bi_2Se_3, Bi_2Te_3. However, the topological property of pure Bi itself is still controversial between theoretical and experimental studies. The tiny band gap and the bulk conduction band minimum located very close to Fermi level at *M* point makes it difficult to directly detect the connection between the surface and bulk bands by ARPES. In this work we approached this problem by using a quantum-confinement effect. In thin film geometry bulk bands are split into so-called quantum-well-state bands, which enable us to observe bulk-like electronic states as clear peaks in photoemission spectra.

The ARPES measurements were performed at NSRRC BL21B1. We used a medium doped p-type Ge(111) wafer as a substrate and confirmed the clean surface by using low energy electron diffraction. Bi was deposited at room temperature and an atomically flat thin film was obtained through post-annealing. This work reports the first ARPES results of Bi thin films on a Ge(111) substrate and we clearly observed surface bands and quantum-well-state bands unique to Bi. Moreover, we systematically observed specific evolution of these bands with the

film thickness, which provides essential information on topological property of bulk Bi.

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■ Invited talk □ Poster

[1] B. Feng, IM, *et al*., Phys. Rev. B rapid comm. *in print*.
[2] S. Ito, IM *et al*., Phys. Rev. Lett. submitted.

Long-range-ordered 2D Tl-Pb Compounds on Si(111) and Ge(111)

Gruznev D.V.,[1,2*] Bondarenko L.V.,[1] Tupchaya A.Y.,[1] Mihalyuk A.N.,[1] Hsing C.R.,[3] Wei C.M.,[3] Zotov A.V.,[1,2] and Saranin A.A.[1,2]

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Since the discovery of graphene the two-dimensional (2D) material science is on the rise due to intriguing properties, which might be present in 2D systems. The (Tl, Pb)/Si(111) system is a vivid example. One of the structures in this system, the binary √3×√3-TlPb reconstruction, has been found to combine a giant Rashba effect and 2D superconductivity [1]. Besides, both Pb/Si(111) and Tl/Si(111) systems individually have displayed advanced properties including superconductivity [2] and spin-polarized valleys [3]. The binary Tl-Pb/Si system has appeared to be rather rich with 2D structures. In the present paper we review the variety of compound surface reconstructions found in the TlPb/Si(111) and TlPb/Ge(111) systems.

In the course of Pb deposition onto the preformed 1×1-Tl/Si(111) surface a series of phase transitions takes place. As Pb partially substitutes for Tl atoms, the formation of √3×√3, 4×4, √13×√13 and 6×6 structures has been observed, depending on Pb coverage and substrate temperature. All the structures have rather common STM appearence, namely a honeycomb lattice with consecutive size enlargement of a unit cell from the smallest √3 to the biggest 6×6. According to proposed model, both elements in these long-range ordered intermetallic compounds are segregated at that compact Pb hexagonal arrays are embedded into a honeycomb lattice that made predominantly by Tl atoms. The same is aslo valid for the Tl-Pb/Ge(111) system, in which √3×√3 and 3×3 structures were observed. Compositions, atomic structures and electronic properties of the compounds have been characterized using combination of LEED, STM and ARPES measurements along with DFT calculations.

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■ Invited talk □ Poster

[1] A.V. Matetskiy, S. Ichinokura, L.V. Bondarenko, A.Y. Tupchaya, D.V. Gruznev, A.V. Zotov, A. A. Saranin, R. Hobara, A. Takayama, S. Hasegawa, Phys. Rev. Lett. **115**, 147003 (2015).

[2] T. Zhang, P. Cheng,W. J. Li, Y. J. Sun, G.Wang, X. G. Zhu, K. He, L. Wang, X. Ma, X. Chen et al., Nat. Phys. **6**, 104 (2010).

[3] K. Sakamoto, T. H. Kim, T. Kuzumaki, B. Müller, Y. Yamamoto, M. Ohtaka, J. R. Osiecki, K. Miyamoto, Y. Takeici, A. Harasawa et al., Nat. Commun. **4**, 2073 (2013).

Superconducting Properties of Tl Double Atomic Layer on Si(111)

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Two-dimensional superconductivity (2DSC) has been studied for a long time. In early experimental demonstrations of 2DSC of ultrathin amorphous films, disorder- and magnetic-field-driven superconductor-insulator transitions (SITs) were intensively discussed in terms of quantum phase transition. Recently, atomically thin 2DSC was realized as superconductiong surface reconstruction such as In/Si(111), Pb/Si(111) and (Tl,Pb)/Si(111)[1]. Since these systems have well-definded crystal and band structures, comprehensive studies by STM, ARPES and transport measurements are in progress.

We report on the first observation of superconductivity in a Si(111)-6x6-Tl using *in situ* electrical resistivity measurements in ultrahigh vacuum. It has been known that this system is “soft" metallic double layer of Tl[2]. In order to explore its ground state, we performed low-temperature elecrical transport measurements. It exhibits a superconducting transition at 0.96 K, accompanied by thermal and quantum fluctuations of order parameter. The system also demonstrates a perpendicular-magnetic-field-induced SIT(Fig.1). Furthermore, we found an intermediate “metallic” state(Fig.1 inset), where resistivity-temperature curves are leveled toward the lowest temperature. An magnetoresitive property at the lowest temperature suggests that the metallicity can be regarded as “Bose metal”, which is a consequence of strong quantum fluctuations.

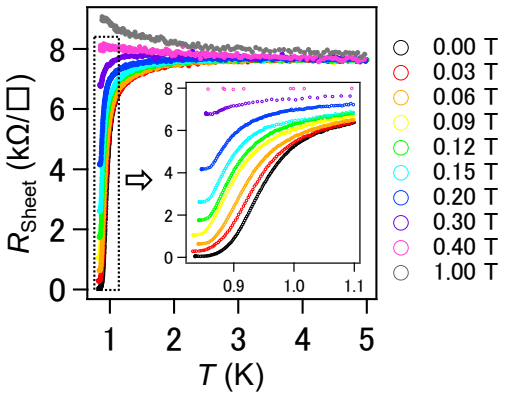

Fig. 1. Temperature dependent sheet resistivity R_{sheet} of Si(111)-6x6-Tl, obtained at 0.00 - 1.00 T. One can see a superconductor-insulator transition around 0.4 T. (Inset) Expanded plot of low-temperature regime. Under small but finite magnetic field, resistivities saturate toward the lowest temperature.

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■ Invited talk □ Poster

[1] A. V. Matetskiy, *et al.* PRL **115,** 147003 (2015).
[2] L. Vitali, *et al.* PRL. **83,** 316 (1999).

Superconductivity and Anomalous Enhancement Induced by Impurities in Two-dimensional Noncentrosymmetric Monolayer $NbSe_2$

Xi Chen

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The noncentrosymmetric monolayer $NbSe_2$ has been successfully synthesized by molecular beam epitaxy on the graphitized SiC(0001) surface. Its electronic band structure and Fermi surface topology have been studied by the angle resolved photoemission spectroscopy, which agrees well with the first principle calculation. The calculation also predicts the lifted spin degeneracy with splitting energy up to 150 meV attributed to the strong spin-orbit coupling interaction. The instability of these two dimensional Fermi surface with spin polarized bands at low temperature has been investigated by using the low temperature scanning tunnelling spectroscopy and a BCS-like superconducting gap has been observed. The superconducting transition temperature was determined to be 0.90 K and the superconductivity of monolayer $NbSe_2$ can be depressed by the perpendicular magnetic field with the magnitude as low as 0.15 T. The possible pairing channels have been discussed in this two-dimensional noncentrosymmetric superconductor. In addition, we observe anomalous superconductivity enhancement induced by impurities.

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■ Invited talk ☐ Poster

MBE Grows of Superconducting β-$PdBi_2$ Films.

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Layered materials (LMs) are built of neutral, single or several atom-thick layers of atoms featuring covalent or ionic connections within each layer without dangling bonds, whereas the layers are held together via van der Waals bonding along the third axis.β-$PdBi_2$ is a superconductor LM which transition temperature equals 5.4 K in bulk form[1]. In addition, β-$PdBi_2$ has recently been found to display nontrivial topological properties[2].

We present the growth method for fabrication of thin β-$PdBi_2$ films with a thickness control that allowed us to grow films from one to dozens layers. The method utilizes MBE deposition of Pd and Bi onto the Bi(111) film grown on Si(111) at room temperature. Structure of the grown β-$PdBi_2$ film was confirmed using low energy electron diffraction (LEED) and scanning tunneling microscopy (STM). Film has three rotational domains due treefold symmetry of the Bi(111) substrate.

Electronic structure measured by angular-resolved photoemission spectroscopy (ARPES) is in good agreement with data, reported for bulk β-$PdBi_2$.[2] Transport properties were measured using van der Pauw method in temperature range from 2K to 300K. The 10 layer films demonstrate a superconducting transition at 3.1 K. Possible reason for lower critical temperature is lower crystal quality of multi-domain film compered to bulk monocrystal.

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■ Invited talk ☐ Poster

[1] Y. Imai, F. Nabeshima, T. Yoshinaka, K. Miyatani, R. Kondo, S. Komiya, I. Tsukada, and A. Maeda, J. Phys. Soc. Jpn. 81, 113708 (2012).

[2] M. Sakano, K. Okawa, M. Kanou, H. Sanjo, T. Okuda, T. Sasagawa, and K. Ishizaka, Nat.Comm. 6, 8595 (2015).

Superconducting Topological Surface States in Non-centrosymmetric Bulk Superconductor PbTaSe2

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§These authors contributed equally to this work.

The search for topological superconductors (TSCs) is one of the most urgent contemporary problems in condensed matter systems. TSCs are characterized by a full superconducting gap in the bulk and topologically protected gapless surface (or edge) states constituted of Majorana fermions. Within each vortex core of TSCs, there exist the zero energy Majorana bound states, which are predicted to exhibit non-Abelian statistics and to form the basis of the fault-tolerant quantum computation. So far, no stoichiometric bulk material exhibits the required topological surface states (TSSs) at Fermi level (E_F) combined with fully gapped bulk superconductivity. Here, we report atomic scale visualization of the TSSs of the non-centrosymmetric fully-gapped superconductor, $PbTaSe_2$. Using quasiparticle scattering interference (QPI) imaging, we find two TSSs with a Dirac point at E≅1.0eV, of which the inner TSS and partial outer TSS cross E_F, on the Pb-terminated surface of this fully gapped superconductor. This discovery reveals $PbTaSe_2$ as a promising candidate as a TSC.

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■ Invited talk □ Poster

[1] Syu-You Guan *et al.*, arXiv:1605.00548 (2016)

Atomic-resolution Simultaneous Imaging of Topography, Surface Potential and Dipole Moment on TiO_2(110) Surface

Haunfei Wen, Yoshitaka Naitoh, Yan Jun Li and Yasuhiro Sugawara*

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Surface potential distributions have been measured using Kelvin probe force microscopy (KPFM) combined with frequency modulation atomic force microscopy (FM-AFM). However, the surface potential distribution measured using KPFM is influenced by the contact potential difference (CPD) between a tip and surface, fixed monopole charges and dipole moment on surfaces and interfaces. Therefore, it is required to distinguish the contributions of dipole moment to the surface potential from those of the CPD and fixed monopoles charges.

In this study, we propose a novel method for measuring the dipole moment on surfaces. This method is based on the measurement of the higher-order nonlinear dielectric effect on surfaces. In the experiments, the higher-order modulation components of frequency shift of a cantilever induced by the ac electrostatic force were used to measure the dipole moment on the surface because of strong distance dependence of modulated electrostatic force and enhancement of the contribution of the short-range electrostatic force [1]. The small-amplitude operation with a stiff cantilever was also used to enhance the force sensitivity and to enhance the contribution of the short-range force associated with the atomic-scale information on the surface. For the first time, we succeeded in achieving atomic-resolution imaging of the topography, the surface potential [2] and the dipole moment on the TiO_2(110) surface using low-temperature FM-AFM [3]. We will discuss the physical origin of the variation of the dipole moment on the surface.

This success is a promising development in the exploration of atomic-scale physical and chemical interactions between atoms/molecules and surfaces and offers deeper insight into the various catalytic processes and functions on surfaces.

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■ Invited talk □ Poster

[1] Z. M. Ma, L. Kou, Y. Naitoh, Y. J. Li and Y. Sugawara, Nanotechnology **24**, 225701 (2013).
[2] L. Kou, Z. M. Ma, Y. J. Li, Y. Naitoh, M. Komiyama, and Y. Sugawara, Nanotechnology **26**, 195701 (2015).
[3] E. Arima, H. Wen, Y. Naitoh, Y. J. Li, and Y. Sugawara, Rev. Sci. Instrum., **87**, 093113 (2016).

How the Phase Transition of Si(111)In-4x1 Proceeds And Is Affected by Various Impurities

Geunseop Lee* and Hyungjoon Shim

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In/Si(111)-4×1 surface consists of an array of In chains, which forms a quasi-1D system. The 4×1 surface at room temperature is metallic but transforms into an insulating 8×2 phase at low temperature below about 125-130K [1]. This temperature-dependent structural and simultaneous electronic phase transition has been found to be of first order [2,3]. The phase transition was shown to be affected by the presence of various impurities (Na, In, H, and O impurities were investigated) [4]. Among them, the influence of the O impurity was found to be exeptional in that it increased the transition temperature (T_c) while the others reduced the T_c.

Here, we will describe some of our past work and address how the phase transitions of both the pristine and impurity-added surfaces proceed in real space. We will also discuss the microscopic mechanisms in which the impurities affect the transition [5,6].

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■ Invited talk □ Poster

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Atomic Structure of Thallium Double Atomic Layer on Si(111)6R3x6R3

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We report on the 1-st observation of superconductivity in a double atomic layer of Tl on Si(111) using in situ electrical resistivity measurements in ultrahigh vacuum. The structure of the Tl bilayer was characterized by a set of techniques, including scanning tunneling microscopy, electron diffraction and photoemission spectroscopy, which concermed the metastability and metallic nature of the Tl bilayer. This “soft” metallic double layer exhibits a superconducting transition at 0.96 K, accompanied by thermal and quantum uctuations of order parameter.

Formation of the double-layer Tl phase takes place when Tl is deposited onto the Si(111)-1x1-Tl surface held at temperatures ranging from RT to about 200_C. It starts preferentially from the atomic steps and spreads over terraces with growing Tl coverage. High-resolution STM observations reveal that the periodic structure is associated with developing of the moire pattern within the array which preserves basic 1x1 periodicity.

We found that double-layer 6x6-Tl phase is consisted of 43 Tl-atoms per layer, and double-layer 6R3x6R3-Tl phase is consisted of 127 Tl-atoms per layer, both are organized as a moire patterns.

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■ Invited talk □ Poster

Metal–Oxide–Semiconductor Plasmonic Nanorod Lasers

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Scaling down semiconductor lasers in all three dimensions hold the key to the developments of compact, low-threshold, and ultrafast coherent light sources, as well as photonic integrated circuits. However, the minimum size of conventional semiconductor lasers utilizing dielectric cavity resonators (photonic cavities) is constrained to the diffraction limit. In the past few years, it has been experimentally demonstrated that the use of plasmonic cavities based on metal–oxide–semiconductor (MOS) structures can break this limit. In this talk, I will report on the recent progress of plasmonic nanolasers using MOS structures. In particular, by using alloy-composition-varied indium gallium nitride/gallium nitride (InGaN/GaN) core–shell nanorods as the nanolaser gain media in the full visible spectrum, we are able to demonstrate full-color nanolasers that can be operated with ultralow continuous-wave (CW) lasing thresholds and single lasing modes. Full-color lasing in these subdiffraction plasmonic cavities is achieved via a unique autotuning mechanism based on a property of weak size dependence inherent in plasmonic nanolasers. As for choice of metals in the MOS structures, epitaxial silver (Ag) films and giant colloidal Ag crystals have been shown by us to be the superior constituent materials for plasmonic cavities due to their low plasmonic losses in the visible spectral range. Recently, we have succeeded in developing InGaN/GaN nanorod array plasmonic lasers based on a metal (Au)-all-around MOS structure, which can be fabricated easily on a wafer scale. I will present the latest results in these new developments.

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■ Invited talk □ Poster

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2D Adsorbate Compounds on Silicon: Experiment versus Theory

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Two-dimensional (2D) multi-component compounds, especially those having one-atom-layer thickness, represent a novel class of 2D materials. Bearing in mind the large number of combinations of atomic species, the number of possible compounds might be quite large and some of them could possess interesting properties. Hypothetical 2D compounds on Si(111) surface have recently become an object in a number of theoretical studies. In particular, it has been theoretically predicted that decorating of Au/Si(111) surface with In, Bi, Tl, Pb, Ge or Sn [1,2] can produce a surface that would exhibits properties of the 2D large-gap topological insulator. The 2D III-V compounds on Si(111) have proposed to possess also the properties of the 2D topological insulators [3,4].

Varification of these predictions is a challenge for experimentalists. Using LEED, STM and ARPES facilities, we have explored a number of the 2D compounds from the above list (e.g., (In, Bi)/Si(111) [5], (Tl, Bi)/Si(111) [6], (Tl, Sb)/Si(111), Au/Si(111) decorated with In, Tl [7,8], Bi and Sn). In these studies, a variety of surface-related phenomena have been disclosed regarding the formation processes of 2D compounds, their structure and properties. However, none of the theoretical predictions have found clear confirmation.

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■ Invited talk ☐ Poster

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Monolayer - Digital Magnetic Alloy (DMA) Formed at the Interface of a-Ge/Mn chain/Si(001)

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Digital Monolayer Alloy (DMA), consists of monolayer of 3d transition metal embedded in group IV semiconductor hosts, has attracted large interested in recent years as a new type material of magnetic electronics, i.e. spintronics [1-3], for example, used as for a spin injection electrode.

We successfully made the DMA by forming 1/2 ML Mn chains on single domain (2 1) surface on stepped Si(001) substrate, by subsequently burying in a Ge layer at RT, with very smooth interface. Ordered structures were characterized with fluorescence X-ray absorption fine structure (XAFS) measurements at the beamline BL37XU, in SPring-8. XAFS data both with polarization along z and along the Mn chain shows no obvious difference between a-Ge/Mn chain/Si(001) and a-Si/Mn chain/Si(001), while that normal to the Mn chain shows different. After the fitting radial distribution function with DFT calculation, we concluded that the obtained structure was a DMA sandwiched between Ge and Si interface, with 0.237-0.238 nm of Mn-Si bonding length. This bond length indicates that Mn stays at a substitution position in Si crystal.

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■ Invited talk □ Poster

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Scanning Tunneling Spectromicroscopy Study on Spintronic Emergent Materials

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We present here the study of scanning tunneling microscopy (STM) with scanning tunneling spectroscopy (STS) on emergent materials with spin characteristics, such as topological insulators (TI), Rashba Semicondutors and hybrids of metal-organic molecules. STS is used to monitor the local electronic structure in nanometer scale for material surface. Rashba semiconductor BiTeI [1] with strong spin-orbit coupling is of great interest for use in spintronic devices exploiting the Rashba effect. Using spatially resolved STS across the lateral boundary between the two terminations, a previously speculated p-n junction-like discontinuity in electronic structure at the lateral boundary is confirmed experimentally.

Further technique by observing quasi-particle interference of the band electrons at BiTeX semiconductor, a hallmark of spin-momentum-locked helical spin texture, beyond only the topological insulators. has been used for extracting the inofrmation on electronic structure with spin characteristics. These findings realize an important step towards the exploitation of the unique behavior of the Rashba semiconductor for new device concepts in spintronics.

Another interesting finding in TI system will be also addressed. Formation of Fe-PTCDA (perylene-3,4,9,10-tetracarboxylic-3,4,9,10-dianhydride) hybrids on the Bi_2Se_3 surface can reveal the functionality of PTCDA to prevent dopant disturbances in the topological surface state, providing an effective alternative for interface designs of realistic TI devices. [2,3] Spin-Polarized STM also observed the spin-response of the organic molecules deposited on magnetic Co islands, which affects the molecular symmetry.[4]

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■ Invited talk □ Poster

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Effect of Chemical Potential Shift on Energy Gap Detection by Scanning Tunneling Spectroscopy

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Scanning tunneling spectroscopy is widely used for local study of the energy structure of surfaces. In many cases such as reconstructed or relaxed semiconductor surfaces, superconductors, topological insulators, the question on presence of the energy gap plays the central role. Differential conductance, $G_d=dI/dV$, of the tunneling barrier is suggested to be a measure of the local density of states, LDOS (see e.g. [1-5] and references therein). Sometime this value is normalized by the tunneling conductance, $G=I/V$. In many cases, zero value of dI/dV is considered as evidence of zero value of LDOS and vice versa, non-zero value of dI/dV is considered as evidence of non-zero value of LDOS. We analyze the effect of shift of the chemical potential on dI/dV [6]. We show, that the effect of the chemical potential shift does not reveal itself only as a voltage shift of the dI/dV curves as a whole. The conclusions mentioned above are correct in the case when the chemical potential level is inside the energy gap. Otherwise, a finite correction of the tunneling junction conductance appears. We derive an expression for this correction, which in a number of cases turns out to be significant and assumes positive (at $V < 0$), as well as negative (at $V > 0$) values. A method of identification and elimination of this correction on the basis of analysis tip-sample separation dependence is proposed.

We demonstrate that the correction δG_d may be important in a number of practically important cases. In particular, non-zero value of dI/dV in the Dirac point observed in the topological insulator Bi_2Se_3 is a good example of such a behavior [7]. In other cases, where the energy gap develops on the Fermi level (superconductivity, charge- or spin-density waves, Coulomb blockade (including dynamical one) *etc*.) zero value of dI/dV corresponds to zero LDOS.

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■ Invited talk ☐ Poster

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Influence of Ferroelectric Polarization on Superconducting Behaviors at $BiFeO_3/YBa_2Cu_3O_{7-\delta}$ Heterointerface

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Multiferroic materials show a wealth of controllable multiple ferroic order through stress, optical excitation, electric, or magnetic fields in the same phase, which in turn suggest potential applications in the realization of oxide-based electronic devices. In multiferroics $BiFeO_3$ system, a large ferroelectric polarization of 90–100 mC/cm^2 is predicted, consistent with the large atomic displacements in the ferroelectric phase. The motivation of this work is to study how the ferroelectric polarization of $BiFeO_3$ modulates the superconducting behavior of $YBa_2Cu_3O_{7-\delta}$ (YBCO) at the ferroelectricity/superconductivity heterointerface. In the past year, we have established a method based on STM and STS measurements in cross-sectional samples to directly elucidate the origin and nature of the local electronic property in heterostructures. In this work, the cross-sectional scanning tunneling results show that the value of the superconducting energy gap 2Δ is smaller when the direction of polarization points to YBCO than pointing away YBCO. The work here directly reveals how the evolution of the superconducting behavior of YBCO is changed by the ferroelectric polarization in $BiFeO_3$.

Keywords: cross-sectional scanning tunneling microscope (XSTM), $YBa_2Cu_3O_{7-\delta}$, $BiFeO_3$, ferroelectricity, superconductivity

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■ Invited talk □ Poster

Sharpness-Induced Energy Shifts of Quantum Well States and Its Applications

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Tip sharpness in scanning tunneling microscopy (STM) can be characterized through the number of field emission (FE) resonances in STM. A higher number of FE resonances indicates higher sharpness [1]. We observe empty quantum well (QW) states in Pb islands on Cu(111) under different tip sharpness levels. We found that QW states observed by sharper tips always had lower energies, revealing negative energy shifts. This sharpness-induced energy shift originates from an inhomogeneous electric field in STM gap. An increase in sharpness increases the electric field inhomogeneity, that is, enhances the electric field near the tip apex, but weakens the electric field near the sample. As a result, higher sharpness can increase the electronic phase in vacuum, causing the lowering of QW state energies.

Moreover, the behaviors of negative energy shift as a function of state energy are entirely different for Pb islands with thickness of 2 and 9 atomic layers. This thickness-dependent behavior results from that the electrostatic force in STM gap decreases with increasing tip sharpness. The variation of the phase contributed from the expansion deformation induced by the electrostatic force [2] in a 9-layer Pb island is significantly greater, sufficient to effectively negate the increase of electronic phase in vacuum..

The sharpness-induced energy shifts of QW states can be applied to distinguish the bonding strength at the film-substrate interface. Further, the effect of the electric field on various types of surface electronic structures such as the surface state, Kondo resonance, and superconducting state can be investigated by tuning the tip sharpness.

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■ Invited talk □ Poster

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The investigation of Local Dipole Moment on TiO_2(110) Surface by Electrostatic Force Microscopy

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Au/TiO_2(110) surfaces display extremely high catalytic reactivity [1]. There are many representative models that explain the emerging catalytic activity of Au nanoclusters. It is widely accepted that the perimeter interface of Au/TiO_2 is the reaction site for CO oxidation. However, the injection/extraction mechanism of electrons and the reaction process are not clarified by a comprehensive experimental description. In this study, we proposed a new method to simultaneously measuring topography, local contact potential difference (LCPD) and dipole moment distribution on TiO_2(110) surface.

In the experiment, the DC bias added with ac bias voltage is applied between the tip and sample. Three lock-in amplifiers are used to detect frequency shift of f_m, f_{2m} and f_{3m}. The contact potential difference is numerically calculated from the divided result of f_m and f_{2m} signals [2, 3] and dipole moment is obtained from frequency shift of f_{3m}. Figure 1 shows the simultaneously measurement result of topography, LCPD and dipole moment images on TiO_2(110) surface. The details will be reported in the meeting.

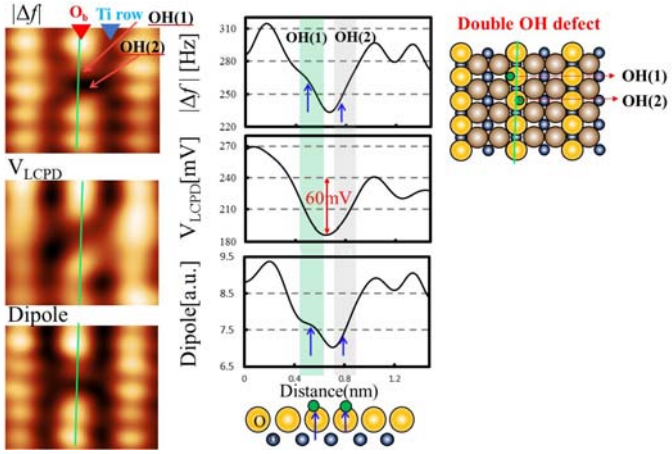

Figure 1. The simultaneously measurement result of topography, LCPD and dipole moment images on TiO_2(110) surface.

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■ Invited talk ☐ Poster

Control of the Dipole Layer of Polar Organic Molecules on Metal Surfaces

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Organic molecules with a permanent electric dipole moment have been widely used as a template for further growth of molecular layers in device structures. Key properties of the resulting organic films such as energy level alignment (ELA), work function, and injection barrier are linked to the magnitude and direction of their dipole layers at the interfaces. Using angle-resolved photoemission spectroscopy (ARPES), we systematically investigate the coverage-dependent work function and spectral line shapes of occupied molecular energy states (MES) of chloroaluminium-phthalocyanine (ClAlPc) grown on Ag(111) thin films of various thickness. We demonstrate that the dipole orientation of the first ClAlPc layer can be altered *via* adjusting the deposition rate and post annealing conditions while it was found that Ag thickness is not a relevant parameter in this regard. The ELA at the interface differs by 0.3 – 0.5 eV between the Cl-up and Cl-down configurations of ClAlPc. Moreover, by comparing the experimental results with density-functional-theory (DFT) calculations based on a realistic model of the ClAlPc/Ag(111) interface, we show that the different orientations of the ClAlPc dipole layer lead to different charge-transfer channels between the ClAlPc and Ag(111), a key factor that controls ELA at the interface and provides a possibility for reliable tuning of the metal work function.

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■ Invited talk □ Poster

Adsorption Chemistry of Aromatic Molecules on Si(5 5 12)

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Comparitive study of organic molecules on Si surfaces provides a variety of adsorption chemistry of the interaction between organic molecules and the Si surfaces. The Si(5 5 12) surface is unique in studying surface chemistry because it consists of various reaction sites such as the dimer, tetramer, adatom, and honeycomb chain. Here we put the molecules of a hexagon ring (benzene, pyridine, and pyrimidine) on the Si(5 5 12) surface and investigate their interaction with the surface using a first-principles calculation. Pyridine and pyrimidine molecules replace carbon atoms with one and two nitrogen atoms, respectively. Because of the hexagonal structure, the overall features of the adsorption structures and energetics are very similar. However, the difference between N and C atoms results in structural and stability variations according to the molecular species. From the atomic and electronic structure analysis, we trace the origins of the different behaviors of the molecules on the surface.

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■ Invited talk □ Poster

Designed Three Dimensional Graphene Architecture

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The fabrications of the 3D graphene networks have made a great advance in graphene research. However, the porous structure of the 3D graphene network cannot be adapted for recent 3D electronic devices, as described below. Recently, 2D electronic devices have moved on to 3D electronic devices with multiple-stacked and/or vertical geometry such as 3D hybrid complementary metal-oxide-semiconductors (CMOSs) or 3D nanoelectromechanical systems (NEMSs). 3D electronic structure has been developed to enhance integration density with overcoming lateral scaling of 2D electronic devices. In addition, the 3D architectures have resulted in better performance, higher connectivity, reduced interconnect delays, low power consumption, better space utilization, flexible heterogeneous integration. To apply graphene to such 3D electronic devices, 3D graphene architecture need to be fabricated in a controlled manner to produce an adaptable 3D graphene structure to other 3D patterned electronic materials in integration process. For this reason, the porous structures of the 3D graphene networks are not appropriate for the 3D electronic devices. Therefore, a different approach to the designed 3D graphene architecture is demanded, which will represent a significant step towards the development of 3D graphene electronic devices.

Here we first demonstrate that 3D designed freestanding graphene architecture can be fabricated in a controlled manner, which can be expandable from the mirco and nanometer scale. A 3D patterned SiC wafer was used to grow a 3D designed freestanding graphene architecture. When the SiC wafer was annealed at a higher temperature of 1650 ºC than a required temperature for regular epitaxial graphene growth, the inside of the 3D SiC architecture was etched with leaving freestanding graphene resembling the 3D SiC architecture, whereas the 3D SiC architecture was fully etched without graphene growth at higher temperatures above 1650 ºC. Interestingly, the 3D SiC architecture was single-crystal, as observed by low energy electron diffraction (LEED). These demonstrate that 3D designed single-crystal graphene architecture can be epitaxially grown by simple, single-step process without further transfer and/or etching process. More interestingly, the 3D designed freestanding graphene architecture was very mechanically sustainable under elastic or plastic deformation, as confirmed by atomic force microscopy (AFM). This mechanical sustainability made electrical current though the 3D graphene architecture reversible under the deformation process, as observed by conducting AFM.

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■ Invited talk □ Poster

Interplay of Charge and Lattice Distortion in Few Layers of Transition Metal Dichalcogenides

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Transition metal dichacogenides have layered structures in the bulk and exhibit various characteristics ranging from normal semiconductors to charge density waves (CDW) to magnetism. Current fabrication techniques have made it possible to extract a single composite monolayer in the laboratory and to measure the physical properties of this truly two-dimensional system. It is also possible to vary the charge carrier density by external gating methods, adding another control parameter to the monolayer configurations. Given these new possibilities, we have performed first-principles calculations to explore the connections among charging, lattice distortion, electronic properties, and charge density waves. In particular, we will report the results for various charge density wave systems in two dimensions and explain the mechanism of forming these phases. In addition, we have also found that substantial hole doping can give rise to a CDW-to-superconductor (SC) phase transition in VSe2.

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■ Invited talk ☐ Poster

Creating Heterointerfaces with Textured Electronic States on Correlated Transition Metal Dichalcogenides

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Domain walls and heterointerfaces in magnetic, ferroelectric, and multiferroic materials have played multiply important roles for various fundamental and technological issues. In this talk, we will review our recent research activity for domain walls and heterojuctions in correlated transition metal dichalcogenides of 1*T*-TaS_2 and $IrTe_2$. Domain walls in the charge density wave (CDW) and Mott insulating state of 1*T*-TaS_2 are thought to be important for metal-insulator transitions, emerging superconductivity, and ultrafast device applications. We discover a method to manipulate domain walls in nanoscale [1] creating a unique heterointerface of correlated metal and Mott-CDW insulator. Two well defined in-gap states are discovered within domain walls [2]. These states are largely determined by strong electron correlation intrinsic to this material, indicating the *internal degrees of freedom within domain walls*. In $IrTe_2$, we discover a new charge ordered state with a hexagonal order and with superconductivity below 3.1 K. It corresponds to a 3q state of 1q stripe orders and forms a heterointerface of superconducting 3q and normal 1q states at low temperature. We will introduce how these systems can further be exploited to synthesize interesting heterointerfaces in vertical direction too by growing epitaxial films on top.

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■ Invited talk □ Poster

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Folding, Stacking and Stitching of Transition Metal Dichalcogenide Monolayers

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Atomically thin two dimensional materials such as graphene and transition metal dichalcogenide are much like sheet papers. They could be folded, stacked or stitched together. However, different from sheet paper, each of two dimensional materials has its own crystal lattice. Depending on how folding, stacking and stitching are done, structural symmetry and ensuing material properties could be greatly tuned. In this talk, I will take an example of transition metal dichalcogenide monolayers to illustrate that the physics behind is fun and intriguing.

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■ Invited talk □ Poster

Electronic Transport and Device Applications of 2D Materials

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During the last decade, tremendous research efforts have been focused on two-dimensional (2D) materials due to their rich physics and great potentials for many applications. Our group at Nanjing University is now focusing on electronic transport, electro-mechanical properties, optoelectronic properties, and related device applications of various 2D materials. My talk will mainly cover our recent studies on transition-metal dichalcogenides (TMD) with low lattice symmetry. In a predicted type-II Weyl semimetal (WSM) material, tungsten ditelluride (WTe_2), we observed notable angle-sensitive negative longitudinal magnetoresistance (MR) and the strong planar orientation dependence which reveal important transport signatures of chiral anomaly. By applying a gate voltage, we further demonstrated that the Fermi energy can be tuned through the Weyl points via the electric field effect; this is the first report of controlling the unique transport properties *in situ* in a WSM system. [1] We also studied atomically thin rhenium disulfide (ReS_2) flakes exhibiting interesting in-plane anisotropic transport and mechanical properties, as well as excellent optoelectronic properties. We fabricated mono- and few-layer ReS_2 field effect transistors, which exhibit competitive performances and record-high anisotropic ratio. We further successfully demonstrated an integrated digital inverter with good performances by utilizing two ReS_2 anisotropic field effect transistors, suggesting the promising implementation of large-scale two-dimensional logic circuits. [2] Our latest results on the ultra-high responsivity phototransistors based on few-layer ReS_2, broadband photovoltaic detectors based on an atomically thin heterostructure and the positive piezoconductive effect observed in suspended multi-layer graphene will also be presented. [3-5]

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■ Invited talk □ Poster

Reversible Manipulations and Detections of Spin-Trans-Effect through Kondo Resonance

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Square organometallic complexes form 6 coordinated structures including two out-of-plane bonds that competes each other; one of the two out-of-plane bonds that formed earlier than the other is weakened with an increased bond length by the formation of the other, which is known as trans-effect. Spin versions of trans-effect has been recently introduced in regard to the coordination reactions between small molecules and metallo-porphyrin on surfaces. They were studied using averaging measurements such as X-ray photoelectron spectroscopy and magnetic circular dichroism, but rarely studied at the single molecule level. Here, we demonstrate that spin interactions in Co-porphyrin/Au(111) can be controlled by coordination and de-coordination of small molecules using scanning tunneling microscopy and spectroscopy (STM and STS). With small molecule coordination, we observed that a zero-bias peak at Co-porphryin, a signature of Kondo resonance in STS, switched off or remained but with a reduced width, i.e., Kondo temperature, and that it could be reversibly retrieved by single molecular STM manipulations. Based on our density functional theory calculation results, the reduced Kondo temperature is explained with the change in the unpaired spins in dz2 orbitals of Co-porphyrin by vertical small molecule coordination. Our study shows that a spin version of trans-effect can be directly probed through Kondo resonance with STS at the single molecule level.

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■ Invited talk □ Poster

Rashba and Dirac States in BiTeX (X = Cl, Br, I) Compounds

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The narrow-gap semiconductors BiTeX (X = Cl,Br,I) have attracted considerable interest because of giant Rashba-type spin-orbit splittings in their bulk and surface electronic states with opposite spin chirality in valence and conduction bands [1–5]. In addition to giant bulk and surface Rashba splitting a single BiTeX trilayer (TL) holds the Rashba-split state itself [6]. The enhanced spin splitting in these materials is driven by their noncentrosymmetric crystal structure in combination with strong atomic spin-orbit coupling and a negative crystal-field splitting of the bands [7]. The latter features have also been predicted to promote a topological insulator (TI) phase in BiTeI under external pressure [8]. An existence of topological surface states has been claimed for BiTeCl at ambient pressure [9], in contradiction, however, to the majority of experimental results. As an alternative route heterostructures between topological insulators and the BiTeX semiconductors have been proposed theoretically [6, 10]. In these heterostructures the interplay of topology and Rashba spin-orbit interaction may give rise to new electronic states and spin-dependent excitation phenomena. Recently we demonstrated that 2D and 3D TI phases can be constructed on the base of BiTeI by the use of stacking of TLs with opposite Rashba spin chiralities [11].

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Atomically Resolved Surface Characterization of the 3-D Dirac Semimetal Cd_3As_2

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Dirac semimetals such as Cd_3As_2 are a recently discovered class of materials which host three-dimensional linear dispersion around point-like band crossings in the bulk Brillouin zone, and hence represent three-dimensional analogues of graphene. This peculiar electronic phase is enabled by specific crystal symmetries: In the case of Cd_3As_2, a C_4 rotational symmetry associated with its unique corkscrew arrangement of systematic Cd vacancies. Although this arrangement underpins the current crystallographic understanding of Cd_3As_2, and all its theoretical implications, it is strangely absent in microscopic investigations reported previously. Here we use a combined approach of scanning tunneling microscopy and *ab initio* calculations to show that the currently held crystallographic model of Cd_3As_2 is indeed predictive of a periodic zig-zag surface superstructure which we observe in scanning tunneling microscopy images. This reconciles the current state of microscopic surface observations with the prevailing crystallographic and theoretical models.

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■ Invited talk ☐ Poster

Dirac Surface States in the Heterostructures of Topological and Trivial Magnetic/Non-magnetic Insulators

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The heterostuctures of magnetic insulator MnSe as well as non-magnetic insulator $SnSe_2$ and topological insulator Bi_2Se_3 were studied by RHEED, STM and ARPES. It was found that films grow epitaxially in all cases at proper parameters. ARPES measurements of Bi_2Se_3 capped with two bi-layers of MnSe revealed that an energy gap of about 90 meV appears at the Dirac point of the original Bi_2Se_3 surface, possibly due to breaking the time-reversal symmetry on the Bi_2Se_3 surface by magnetic proximity effect from MnSe [1]. In case of Bi_2Se_3 capped with $SnSe_2$ overlayer the Dirac surface states stay intact. One triple layer of $SnSe_2$ was found to be an efficient spacer for separating a Bi_2Se_3 topological-insulator slab into two and creating the corresponding topological surface states.

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A Metal-Insulator Transition of the Buried MnO_2 Monolayer in Complex Oxide Heterostructure

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Due to the interplay of lattice, charge, orbital, and spin degrees of freedom, strongly correlated electron systems in complex oxides generate a rich spectrum of competing phases and emergent physics. Recently, extensive studies suggest that complex oxide interfaces provide a powerful route to manipulate these degrees of freedom and offer new possibilities for next generation devices, thus create a new playground for investigating novel physics and the emergence of fascinating states in condensed matter. In 2004, a two-dimensional (2D) electron gas was discovered at the $LaAlO_3/SrTiO_3$ (LAO/STO) heterointerface. On the other hand, the discovery of free-standing 2D materials has inspired the research for exploring new low-dimensional materials. Pioneered by graphene, these 2D materials exhibit aboundant unusual physical phenomena that is undiscovered in bulk forms. The confinement of charge and heat transport at such ultrathin planes offers possibilities to overcome the bottleneck of current devices. Interestingly, in complex oxides, the physical properties have usually been dominated by their 2D structural units, the metal-oxide planes. However, most studies about understanding the contribution of such oxide planes on the corresponding properties still concentrate on the viewpoint from their macroscopic behaviors in bulk materials. Therefore, to create and manipulate a single metal-oxide plane would provide other solutions for realizing the fundamental physics of the strongly correlated electron systems. In this talk, I attempted to create a single metal-oxide plane as a 2D monolayer through interface engineering. This 2D oxide monolayer can be obtained at the heterostructure similar to the case of a single-unit-cell manganite ultra-thin film sandwiched between two neighboring complex oxides.[19] In such heterostructures, the intrinsic properties of 2D oxide monolayer can provide a basic understanding of the physics on the dimensionality-confined strongly correlated electron systems. This study delivers a generic approach to study the dimensional confinement of strongly correlated electron systems and provides a direction to design new electronic devices.

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■ Invited talk □ Poster

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Growth of Ge and Si on the Monolayer Silicene on Ag(111)

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Growth of Ge by molecular beam epitaxy on top of silicene monolayer on the Ag(111) surface results in either a dispersed adlayer or a two-dimensional ordered depending on the silicene phases. Scanning tunneling microscopy (STM) images show that the ordered adsorbed Ge atoms on the domains occupy directly on top of down-atoms in the buckled silicene layer. By contrast, further growth Si on the silicene up to several MLs results in an atomic flat film with $(\sqrt{3} \times \sqrt{3})$ surface structure. We use low-temperature scanning tunneling microscopy (LT-STM) to observe the chemical response of the film surface exposed to an atomic deuterium (D) beam. We find D displaces the Ag surfactant adatoms, resulting in a D-terminated (1 × 1) surface. The displaced Ag atoms migrate on the surface to form Ag(111) crystallites. The results confirm that the surfaces of the few-layer Si films grown on Ag(111) are Ag terminated and suggest that the films have a diamond-like structure [1].

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■ Invited talk ☐ Poster

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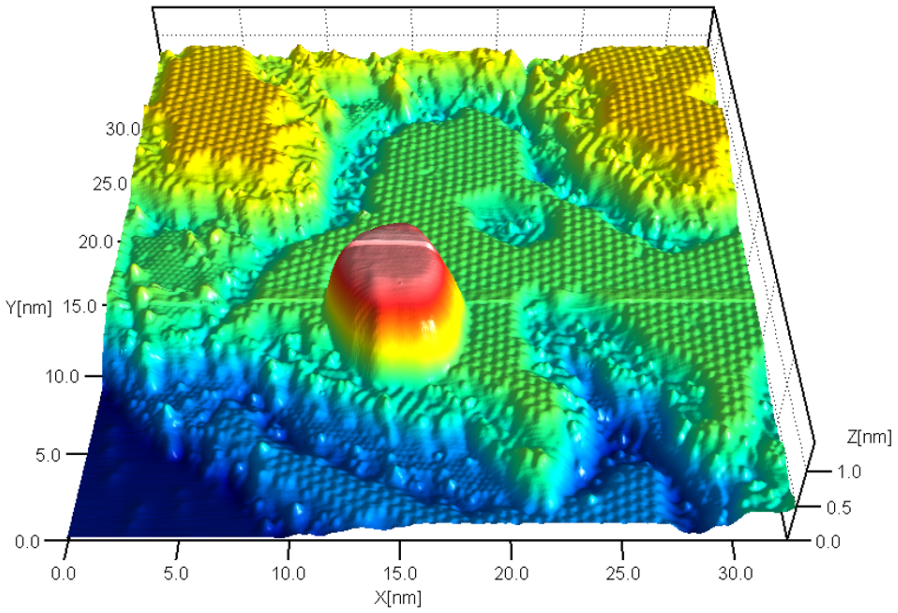

Thermoelectric Imaging of Structural Disorder in Epitaxial Graphene with Atomic Resolution

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Heat is a familiar form of energy transported from a hot side to a colder side of an object, but not a notion associated with microscopic measurements of electronic properties. A temperature difference within a material causes charge carriers, electrons or holes, to diffuse along the temperature gradient inducing a thermoelectric voltage. Recently, we have demonstrated that local thermoelectric measurements can yield real-space images of local electronic density of states (LDOS) and structural disorder in epitaxial graphene on the atomic and nanometer scales [1,2]. The thermoelectric measurement acts to amplify the variations in LDOS at the Fermi-level, giving high differential contrast in thermoelectric signals. Using this imaging technique, we uncovered the dimensional evolution of disorder in epitaxial graphene, which is the evolution of strain-response patterns with increasing thickness: spot, line, and domain patterns. Disorder and strain can have large and spatially localized electronic signatures, even for subtle changes in atomic positions. We detect these signatures by exploiting thermopower that reflects distortions in the electronic structure, which enabled us to image the structural change due to strain.

Because thermoelectricity, or Seebeck effect, is associated with heat-induced electron diffusion, how the thermoelectric signal is related to the atomic-scale wavefunctions and what the role of the temperature is at such a length scale remain very unclear. Regarding the questions, we showed that coherent electron and heat transport through a point-like contact produces an atomic Seebeck effect, which is described by mesoscopic Seebeck coefficient multiplied with an effective temperature drop at the junction interface. The mesoscopic Seebeck coefficient is approximately proportional to the logarithmic energy derivative of local density of states at the Fermi energy. We deduced that the effective temperature drop at the tip-sample junction could vary at a sub-angstrom scale depending on atom-to-atom interaction at the interface. A computer-based simulation method of thermoelectric images is proposed, and a point defect in graphene was identified by comparing experiment and the simulation of thermoelectric imaging.

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■ Invited talk □ Poster

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Dual-Phase Single-Layer Germanene on Ag(111)

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Two distinct phase-separated single-layer honeycomb germanene lattices were identified for germanium growth on Ag(111). The geometric and electronic structures of these two phases, and their correlations, were characterized by scanning tunneling microscopy, low energy electron diffraction, angle-resolved photoemission, and ab-initio calculations. We discovered that a "stripe phase" germanene, which is partially commensurate with Ag(111) and possesses significant tensile strain, exhibits the unambiguous atomic up-down buckling pattern of an ideal germanene lattice. This stripe phase emerges from the de-alloying process of the known Ag2Ge surface alloy phase and covers the whole surface at 0.84 monolayer (ML) of Ge. Up to 1.08 ML, a new strain-relaxed germanene phase, which shows an abrupt decrease of Ge-Ge bond length to that of free-standing germanene and is fully incommensurate with Ag(111), appears and coexists with the stripe phase. This denser germanene phase is "quasi-free-standing-like" because it preserves the electronic structure symmetry at germanene $\overline{K}$ point and the dominant band observed at –3.5 eV, corresponding to Ge-Ge σ bonding, decouples itself from the Ag bulk bands. In contrast, the electronic structure of the stripe-phase germanene diminishes at the germanene $\overline{K}$ point and a new band coupled strongly to the substrate emerges at the Ag(111) Mbar point. In both cases, experimental results are consistent with theoretical calculations. Dual germanene phases on a single substrate provides an unique opportunity for us to compare the electronic and geometric structures of two honeycomb germanene lattices therefore to elucidate the structure-property correlation therein.

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■ Invited talk □ Poster

Dependence on Size of Supported Rh Nanoclusters in the Decomposition of Methanol

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The catalytic decomposition of methanol is extensively investigated because the principal reaction is applied in direct methanol fuel cells (DMFC), which offer a prospect of efficient conversion of methanol to electricity, and because it can serve as a source of hydrogen. As the performance of DMFC or the production of hydrogen is governed largely by the catalyzed reaction, a knowledge of the detailed reaction kinetics and a correlation between reactivity and structure of the catalysts are desirable. Many model systems, including single-crystalline metallic, alloy and oxide surfaces, have been investigated to shed light on the mechanism of the reaction and to correlate reactivity with structure. However, methanol reactions on oxide-supported clusters, a realistic model system, have been little investigated. The present work has an aim to remedy this lack. We investigated the decomposition of methanol and methanol-d_4 on Rh clusters supported on an ordered thin film of Al_2O_3/NiAl(100), under UHV conditions and with various surface probe techniques. Methanol on Rh clusters decomposed via dehydrogenation to CO; the production of CO and hydrogen (deuterium) per Rh surface site varied notably with the cluster size. For Rh clusters of diameter $<$ 1.5 nm and height $<$ 0.6 nm, the production increased with decreasing size of the cluster, up to four times that on the large clusters or Rh(100) single crystal surface. The reactivity was enhanced largely because, with decreasing cluster size, the activation energy for the scission of the O-H bond in the initial dehydrogenation became smaller than the activation energy for the competing desorption. The property was associated with the corner Rh atoms at the surface of small clusters.

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■ Invited talk □ Poster

Unveiling Microscopic Structures of Charged Water Interfaces by Surface-Specific Vibrational Spectroscopy

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Charged water interfaces are ubiquitous and responsible for many important processes in nature and modern technologies, such as protein folding, electrochemistry, and photocatalysis. They appear in the form of an electric double layer that can be divided into two sub-layers. One is the so-called Stern layer composed of one to two hardly mobile, hydrogen-bonded, water monolayers next to the charged plane. The other is the diffuse layer, in which ions assuming the Poisson-Boltzmann distribution set up a dc field distribution. Being directly associated with the charged surface, the Stern layer directly controls the microscopic energy transfer and chemical reaction pathway at the interface. However, despite extensive studies on charged water interfaces, current knowledge on the microscopic structure of the Stern layer is still extremely limited. The difficulty lies in the inability of existing techniques to selectively extract structural information about the Stern layer in the presence of the diffuse layer. We now have developed a sum-frequency spectroscopy method that allows us to obtain the vibrational spectrum, and hence the microscopic structural information, of a Stern layer. Application of the method to a prototype lipid (fatty acid)–water interface reveals significant variation of its Stern layer structure upon deprotonation of the lipid headgroup. The measurement also yields a spectrum that characterizes the dc-field-induced sum-frequency generation from bulk water in general, and can help to deduce vibrational spectra of the Stern layer of other charged water interfaces. This unique ability of our method provides opportunities to gain better microscopic understanding of properties and functionality of charged water interfaces.

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■ Invited talk □ Poster

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√7×√7-AuTl compound surface structure on Si(111)

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2D multicomponent structures start attracting a considerable attention as they might exhibit unique properties, which are not observed in the bulk counterpart. The number of reported 2D compounds is growing, including thallium-based ones. Tl is valued for its strong spin-orbit coupling. Besides, Tl can be easily replaced from the equilibrium positions on Si surface at relatively low temperatures [1] baring the unreconstructed Si(111) and allowing easy creation of new binary materials. Using this approach a number of novel structures have been created [1, 2]. Interest in an AuTl low-dimensional compound is motivated by the study that shows drastic changes in electronic and structural properties of Au-induced reconstruction modified with small amount of Tl (~0.15 ML) [3].

Au deposition at RT onto the pre-formed Tl/Si(111) surface leads to the development of well-ordered AuTl layers with 2√7×2√7 periodicity . With further Au deposition a next structure develops having √7×√7 lattice and the composition close to AuTl. When this layer uniformly covers the entire surface the total metal coverage is estimated to be about 3 ML (~1.5 ML of Tl and ~1.5 ML of Au). The binary AuTl layer has a perfect long-range order as revealed by means of STM and LEED analysis. In STM images this reconstruction appears as hexagonal array of clusters with a bright core and six surrounding protrusions. ARPES spectra collected using He-Iα light revealed the metallic nature of the surface; its band structure consists of a complicated mixture of parabolic bands and small electron pockets crossing the Fermi level. The formation process and the plausible structure of atomic arrangement are discussed.

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☐ Invited talk ■ Poster

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The Study of Silicene Growth on Ag(111)/Si(111) Surface

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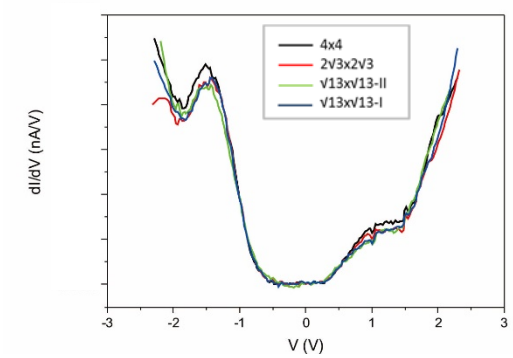
Silicene, the two dimensional monolayer films and the same group IV element with graphene, is expected for its abundant properties. However, the difficulty of structure growth and the demand for special substrates limit the possibility of further applications. Using scanning tunneling microscopy (STM) and scanning tunneling spectrum (STS), the formation of silicene on the 6~12ML Ag (111) thin films was studied. The Ag films were pre-grown on the Si (111) substrates. The classical silicene superstructures, such as 4×4, √13×√13, 2√3×2√3, can be observed on this Ag (111) thin film covered Si(111) surfaces. The more continuous silicene sheet formed on 6~12 ML Ag (111)/Si(111) substrate than on the single crystal Ag (111) surface. Various silicene superstructures are usually discontinuous on the single crystal Ag (111) surfaces, but continuous on the thin film Ag (111) surfaces by Ag domain rotation on Si (111) surfaces. A flexible thin film Ag (111) surface seems a better substrate than solid crystal Ag (111) for silicene growth. The STS of each superstructure of silicene was measured and found the similar electron properties as the following figure. It indicates the possible application for multi-superstructure silicene.



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☐ Invited talk ■ Poster

Step Edge Effects in the Topological Insulator Bi_2Se_3 Revealed by Scanning-Tunneling Spectroscopy

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Topological insulators have been attracting much attention recently as a class of materials possessing intriguing physical properties and because of their potential applications in spintronics [1]. 3D topological insulators are band insulators in the bulk, but have topologically protected surface states (SS) that span the whole bulk band gap. In the case of topological insulator Bi_2Se_3 these states form a single Dirac-like cone in the momentum space with its apex (Dirac point, DP) located in the bulk band gap.

Here we present results of detailed study of the topological insulator Bi_2Se_3 surface state energy structure in the vicinity of surface steps by means of scanning tunneling microscopy (STM) and spectroscopy (STS) [2]. An increase in the chemical potential level in the vicinity of step edges is observed. The value of the chemical potential growth (0.1-0.2 eV) is found to correlate with the step height and is caused by redistribution of electron wave functions between outer and inner edges of surface steps, as it is known for usual metals [3]. Smaller value of the shift and its larger characteristic length in comparison with the usual metals reflect specifics of the helical surface states. The growth is accompanied by an increase in the differential tunneling conductance, dI/dV, in the helical surface states energy region and thereby produces illusion of appearance of the edge states. We show that this tunneling conductance growth is reproduced in the framework of a tunneling model taking into account the tunneling gap transparency dependence on apllied voltage [4].

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☐ Invited talk ■ Poster

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Optical-Helicity-dependent Photocurrent in Strong Spin-Orbit Coupling Thin Films Grown on Si Subatre

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When we shine circulary polarized light onto a sample such as quantum wells with spin-orbit interaction [1], topological insulators [2] and spin-valley coupling systems [3], photocurrent is induced even without bias volatge applied across the sample and the current direction is reversed with change in helicity of the light. This phenomenon of optical-helicity-dependent photocurrent is usually ascribed to so-called circular photogalvanic effect (CPGE) in which electrons having a particualy direction of spin are preferentially excited and flow in a direction parependicualr to the spin direction because of so-called spin-momentum locking. When the helicity of the iluumination light is reversed, electrons of the opposte spin are preferentially excited (selection rule) so that the photocurent direction is revsersed. This zero-bias photocurrent is said to be spin polarized because of the preferential excitation of one-spin electrons by circualry polarized light as mentioned above, thus it is promised to be of great use to spintronic devices.

So far, however, no such phenomenon has been reported in surface Rashba systems in which the spin splitting in surface-state bands and spin-momentum locking occur. Our initial purpose was to invistigate the posibility of CPGE in surface Rashba systems. In our experiment, we observed a light-polarization dependent photocurrent with visible lasers by *in situ* measuring the photovoltage across samples such as Bi(111), Bi/Ag(111) and Bi_2Se_3(111) thin films grown on Si(111) substrate in ultrahigh vacuum. By measuring the dependence of the photovoltage on the light incident angle and comparing it with the reflectance of light, we confirmed that what we observed cannot be explained by the phenomenological theory of CPGE. We suggest that this photocurrent arises from the process as follows: 1. Spin imbalance in the excited electrons is generated by the circularly polarized light illumination according to the selection rule. 2. Via the Inverse Rashba-Edelstein effect or Spin Galvanic effect, this nonzero spin density is converted into electrical current which is not spin-polarized.

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The Adsorption and Desorption of Water on MgO(100): the Application of Random Structure Searching Method

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The adsorption and desorption of water on perfect and defect MgO(100) surfaces are studied using random structure searching (RSS) method [1] which has been shown to be efficient and effective for the structure searching [2, 3]. In contrast to the previous studies, we obtain the adsorption and desorption structures and find possible adsorption/desorption processes using the RSS method without introducing any constraints. The reaction pathways for water desorption from MgO(100) surface will be discussed.

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First-Principles Calculations of $BiFeO_3$ Surface/Water Interaction

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Since the discovery of water splitting phenomena using TiO_2 and Pt electrodes by Fujishima and Honda [1], hydrogen production via photocatalytic water splitting is one of the important developing technologies for realizing Sunlight energy harvesting [2]. To have high efficiency of hydrogen production, several dynamic processes including generating photo-excited electron-hole pairs, reducing electron-hole recombination, and backward reaction are the major considerations in the design of photocatalysis system.

At room temperature, $BiFeO_3$ (BFO) possesses ferroelectric polarization beyond 50μC/cm^2 along the [111] direction; the corresponding built in electric field is helpful to separate photo-excited electron-hole pairs [3,4]. On the other hand, the bandgap of BFO (2.3 to 2.8 eV) is suitable for visible light absorption that surpassing many traditional photocatalysts like TiO_2, ZnO with wide bandgap greater than 3 eV. Recently, several works had demonstrated using BFO in photovoltaic applications [5,6] which supports the idea of using BFO as a feasible photocatalyst for hydrogen production with switchable properties [3,4].

Based on density functional calculations, we have modeled the processes for one water molecule splitting on BFO (001), (011), and (111) surfaces. It is found that three surfaces have different activities on promoting water splitting. The (111) surface promotes water splitting most, and then the (011) surface with water splitting states lower than the intact water states in terms of energy. On the other hand, the water splitting state and intact water state are almost equivalent on (001) surface. The up and down polarizations will affect the water splitting in different degrees on surfaces but the chemical conditions of surfaces (surface terminations) seem more important to the polarization directions. The projected surface density of states is also analyzed to inspect how surface states can assist the separation of electron-hole pairs.

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Photoinduced Band Alignments and Carrier Generations at PbI_2/Perovskite Interface of Perovskite Solar Cells

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The presence of PbI_2 in perovskite films has been found to affect the charge carrier transport behaviors and device performance of perovskite solar cells. The scanning tunneling microscopy (STM) combined with spectroscopy (STS) has demonstrated the unique ability to provide the direct and local information of topography and interfacial band structure in organic[1], oxide[2,3] and semi-conductor systems[4]. In this work, we employed a novel light-modulated scanning tunneling microscopy (LM-STM) technique to reveal the correlation of the nanoscaled compositional distributions and interfacial electronic structures at the PbI_2/perovskite interface of polycrystalline $CH_3NH_3PbI_3$ perovskite grains under light illumination. Most importantly, this technique enabled us to directly obtain the spatially-resolved mapping images of photogenerated electron and hole carriers and the photoinduced interfacial band bending of both the valence bands and conduction bands at the PbI_2/perovskite interface of perovskite crystals for the first time.

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Band Alignment Across 1D WSe_2-$MoSe_2$ Heteroboundary

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Monolayer transition metal dichalcogenides (TMDCs) have appeared as promising successors of graphene, the most famous two-dimensional (2D) material with exotic structural and electronic features. In monolayer 1H TMDCs composed of group VI metals, existence of band gaps and spin-valley interactions are useful for electronics, spintronics, and valleytronics. Functionalities can be further expanded *via* heterostructures. For example, lateral TMDC heterojunctions have exhibited potential in optoelectronics.[1] However, detailed studies at the boundaries of these 2D heterojunctions are essential but still rare. We performed scanning tunneling microscopy (STM) and spectroscopy (STS) at room temperature to investigate a WSe_2-$MoSe_2$ heterojunction on HOPG. We find that $MoSe_2$ and WSe_2 share the same lattice orientation and moiré patterns are observed on both surfaces. Across the heteroboundary, a narrow and symmetric depletion region of few nanometers exists, from which large electric fields as well as high carrier density can be derived. Our work reveals the band alignment at the nanoscale for a lateral TMDC heterojunction, which can help to enlarge TMDC application designs.

☐ Invited talk ■ Poster

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Two-Dimensional Molybdenum Nanomaterials Based DNA Sensors

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We have developed a two-dimensional (2-D) materials based DNA sensors. The molybdenum series of 2-D nanosheets (MoO_3, $MoSe_2$, MoS_2, and $MoTe_2$) play an excellent sensing platform towards the DNA detection. Herein, we report the DNA sensing of prostate-specific antigen (PSA) with a very high sensitivity and selectivity by using fluorescence techniques. The DNA sensor system is designed based on the mechanism of fluorescence turn-off/on. Fluorescence sensing studies reveal that the MoO_3 system exhibits a detection limit of ~11 pM which is much higher sensitivity compared to that of other reported DNA sensors systems [1,2]. Though other 2D nanosheets $MoSe_2$, $MoTe_2$ and MoS_2 also possess better sensitivity towards the detection of DNA. For practical application, the sensing capabilities of DNA in the live cells were performed and the confocal fluorescence images (*in vitro* bioimaging) results revealed their promising applicability as an effective and non-toxic DNA sensors.

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Thermal Evolution of Iron on Ge(111)-c(2x8) and Ag/Ge(111)-(√3×√3) Surfaces

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We deposited iron atoms at room temperature on Ge(111)-c(2×8) substrate less than one monolayer and anneal at different temperatures. By using scanning tunneling microscope the thermal evolution was investigated. STM images show that iron will cause defects and holes on substrates at room temperature. As the annealing temperature rises, iron atoms pull out germanium to form some kinds of alloyed islands. On the other hand, Fe on Ag/Ge(111)-(√3×√3) shows that silver can protect the (√3×√3) reconstruction from forming defects, but substrate is still pulled out at high annealing temperatures. The kinds of islands in Fe/Ge system are similar with Fe/Ag/Ge system, but a few differences show that silver still affects the development of islands.

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☐ Invited talk ■ Poster

Low-Voltage Electric-Double-layer Organic Transistors with Polar Rubbery Dielectrics

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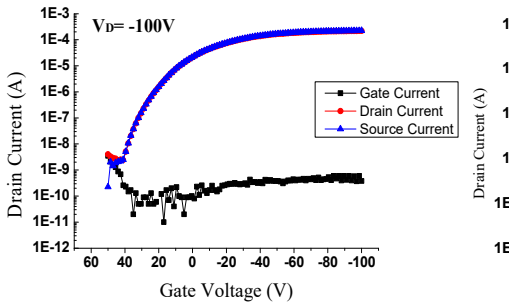
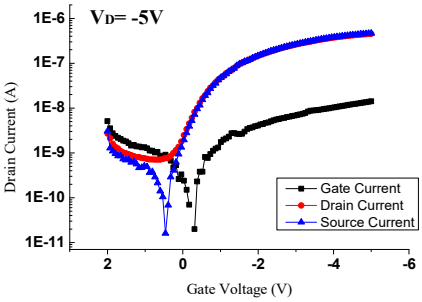
In recent years, organic semiconductors have been widely used on practical applications. The organic transistors at low operation voltages are favorable for electronic applications or sensors. At first, we have demonstrated that soultion coating of 6,13-bis(triisopropylsilylethynyl) pentacene (TIPS-pentacene) offers good air-stable and great mobility about 0.8 $cm^2V^{-1}s^{-1}$ on SiO_2 substrate. We used blade-coating to form a high degree of morphology control of thin-films. However, such devices showed high operation voltages of -100V. It is not suitable for applications.

In order to improve the problem, we describe the electric-double-layer effect in polar rubbery dielectrics. Zhenan Bao (2015) indicated the polar elastomer poly(vinylidene fluoride-co-hexafluoropropylene) (e-PVDF-HFP) being as the dielectric layer allows low operation voltages[1]. In the case of e-PVDF-HFP, electric-double-layer charging effect is related to its low Tg (~ -20ºC) and the high polarity. It is well known that elastic polymers are desirable matrixs fot ion conductors due to the segmental motion that facilitates ion transport. In our work, we substituted e-PVDF-HFP for SiO_2 by spin-coating and thermal curing at 180ºC for 6 hours. In Fig.3, there are some divided nanoparticles on PVDF surface. Hence, we assume that the PVDF thin film is composed of nanoparticles with an amorphous structure, which is favorable for proton conduction. Our results show that TIPS-pentacene semiconductors can be operated at low-voltages and be air-stable over one month with e-PVDF-HFP.





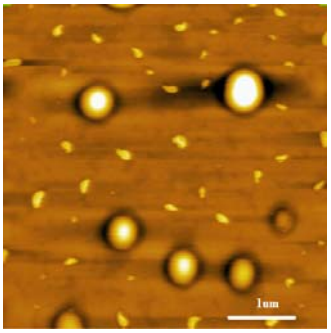


Fig.1 Device characteristics on SiO_2. Fig.2 Device characteristics on e-PVDF-HFP. Fig.3 AFM of PVDF thin film.

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Amorphous Metal Oxide TFT with EDL Controlled Performance

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Semiconducting amorphous metal oxide thin film transistors (TFTs) are considered as the potential candidate of next generation optoelectronic device due to their superior performance compared with organic and amorphous silicon based TFT. Despite all the merit of metal oxide based TFTs, the high operating voltage, and requirement of high annealing temperature still are some of its major downsides. In past few years, electric-double-layer (EDL) metal-oxide TFTs have been proposed to ameliorate these issue owing to the high capacitance at gate dielectric[1]. Nevertheless, these previous works all base on vacuum process which is difficult to achieve low cost electronics[2]. Thus, an approach to integrate solution process fabrication with electric-double-layer (EDL) metal-oxide TFTs is needed.

In this article, we propose a solution processed high performance a-IZO electric-double-layer transistor (EDLT) gate with CYTOP fluoropolymer dielectric, and investigate its electric characteristic by comparing conventional SiNx bottom gate configuration with CYTOP top gate configuration as shown in figure 1. In Figure 1, the field effect mobility and subthreshold swing of three different device which were annealed at same condition, SUT annealing at 200 °C 30 min. The top gate CYTOP dielectric devices show a huge reduction of operation voltage (<3V), a significant improvement (the factor of 20) of mobility (34.6 $cm^2/V{\cdot}s$), and a lower subthreshold swing.

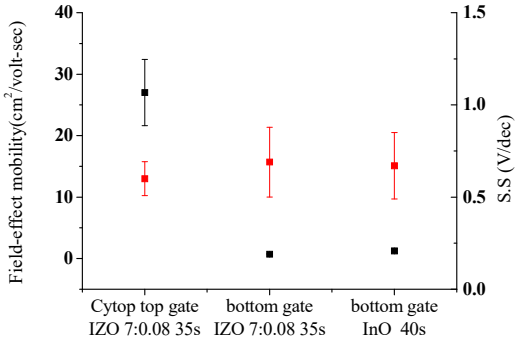

Figure 1. Field effect mobility and subthreshold swing plot with different configuration devices

This result showed that our a-IZO electric-double-layer transistors (EDLT) are very promising for low-cost high performance optoelectronic application.

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Theoretical Study of Quantum Size Effects in Thin Al(100), Al(110) and Al(111) Films

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We have carried out first-principles calculations of Al(100), Al(110), and Al(111) films to study the oscillatory quantum size effects exhibited in the surface energy, work function, electron-phonon coupling constant λ and transition temperature Tc of superconductivity. Significant oscillatory quantum size effects are found in these quantities. These oscillations are correlated with the thickness dependence of the energies of confined electrons, which can be properly modeled by an energy- dependent phase shift of the electronic wave function upon reflection at the interface. It is found that a quantitative description of these quantum size effects requires full consideration of the crystal band structure.

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Measurement of Work Function and Instability of Field Emission Current of Inert Gas Adsorption on Nb(100)

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We show that Nb {100} is a good electron source. We fabricate a thermally stable pure niobium tip with a small {100}facet faceting structure surrounded by four {310} surfaces by thermal treatment in UHV. We can observe the structure of the tip by field ion microscopy (FIM) and measure the characteristic of field emission electron beam by field electron microscopy (FEM).

In order to enhance electron current, we expose the tips under various gas (Ne, Xe) environment (Langmuir).The variation of field-emission work functions due to different gas absorption can be calculated from the Fowler-Nordheim plots. We find the best exposing environment for different gas (Ne, Xe) and measure the stability of the field emission current from niobium {100} facet with Faraday cup in 30 minutes.

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☐ Invited talk ■ Poster

Electronic Structures of Heusler Compounds Including Many-Body Effects

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To investigate electronic structures of Fe-based and Ru-based Heusler compounds, we have performed DFT calculations using PBE and HSE06 hybrid functional. In the PBE calculations, Heusler compounds were semimetals or nearly-gapless semiconductors; however, in the HSE06 calculations, Fe-based Heusler compounds were semiconductors and Ru-based Heusler compounds were narrow band-gap or nearly-gapless semiconductors. It reveals that the electronic structures in DFT level have strong exchange-correlation functional dependence and thus the many-body corrections are needed. The quasiparticle GW approximation [1-2] including a proper many-electron screening effect was then carried out to study these Heusler compounds.

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Material Simulation by Using Random Structure Searching

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Random structure searching (RSS) [1] has been proved to be a powerful approach to search the stable crystal structures. A true random sampling is known to be trustworthy yet highly time-consuming to find the global minimum. Thus the implementation of reasonable constraints has become one of the most essential issues in the approach. We therefore propose both the symmetry-related constraint and the concept of an object which can succesfully improve the efficiency of the method. Several representative materials are examined, including molecular crystal (methanol) [2], high-pressure carbonates ($MgCO_3$, $CaCO_3$) and Si(111)-5X5 surface structures to demonstrate the advantages of the symmetry-related RSS method.

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Simulation Study of $EuVO_4$ Under High Pressure

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$EuVO_4$ is a member of RVO_4 family (R for "rare" earth element), which have attracted lots of attention due to their intriguing properties and some potential applications. This kind of materials have been studied both experimentally [1, 2] and theoretically [2, 3] below 35GPa. It has been confirmed that there are three different phases in the range from ambient pressure to 35 GPa. However, to our knowledge, no experiment data are available for this kind of materials under higher pressure, and no one has applied a systematic structure search to study the RVO_4 family.

Our goal is to find an efficient way, without loss of the generality, to extrapolate the structures of $EuVO_4$ under different pressures. The basic idea of our approach is using *ab initio* Random Structure Search (AIRSS) [4], published in 2011 by Chris J. Pickard and R. J. Needs. Furthermore, we want to take this case as an example to set up a SOP to study many different materials which have more complicated chemical formula like $EuVO_4$ in our case. At the present stage, our results show that the proposed method can work efficiently and successfully.

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☐ Invited talk ■ Poster

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