# ISSP ワークショップ

第5回伊藤国際学術研究センター会議(IIRC-5)「Forefront of Molecular Dynamics at Surfaces and Interfaces: From a Single Molecule to Catalytic Reaction」の報告

### 東京大学物性研究所 告信 淳

本国際会議は、平成 29 年 11 月 20 日から平成 29 年 11 月 23 日の 4 日間、東京大学伊藤国際学術研究センター基金、理化学研究所 100 周年記念事業、ISSP 国際ワークショップ、ISSP ワークショップの支援を受け、表面界面スペクトロスコピー研究会との共催により東京大学本郷キャンパス内の東京大学伊藤国際学術研究センターで行われた。実行委員会の委員長は、吉信淳(物性研究所)、副委員長は金有洙(理化学研究所・主任研究員)、委員は、増田茂(東京大学・大学院総合文化・教授)、渡邉聡(東京大学・大学院工学系・教授)、福谷克之(東京大学・生産研・教授)、高木紀明(東京大学・大学院新領域・准教授)、中村潤児(筑波大学・教授)、米田忠弘(東北大学・多元研・教授)、荒船竜一(物質材料研究機構・主任研究員)である。

本国際会議のスコープである表面および界面における分子のダイナミクスを理解することは、基礎科学から応用分野に及ぶ広範な研究分野においてますます重要性を増している。表面および界面は、材料におけるエネルギーや物質の移動において重要な役割を果たす。幅広い産業分野におけるナノテクノロジーの応用は、様々な特性を有するナノスケール材料および低次元原子層材料の探索を促進している。さらに、走査プローブ顕微鏡、シンクロトロン放射光およびレーザーによる分光、第一原理密度汎関数理論計算

などの実験および理論の進歩により、原子・分子レベルで 表面における過程を解明し制御できるようになった。

本国際会議は、具体的に以下のような表面界面における分子ダイナミクスに焦点をあて、シングルセッションの 口頭発表とポスター発表が行われた。

- ・吸着単分子の物理と化学
- ・表面界面における低次元物質
- ・モデル触媒における動的プロセス
- ・表面界面におけるデバイスの分子プロセス
- ・固液界面における素過程

参加者は、196名(招待講演 30名、一般口頭発表 13名、ポスター発表 109名を含む)であった。その内、国内からの参加者は 133名(うち、招聘者 19名)、国外からの参加者(うち、招聘者は 15名)は 63名であった。

国内外の著名な研究者による招待講演、活躍中の中 堅・若手研究者による一般講演、およびレベルの高いポス ター発表に対して、活発な質疑応答が行われた。会期中、 休憩時間や食事の際も、熱心に意見交換が行われた。開催 中および会議後、参加者から会議の運営と内容について多 くのポジティブな意見をいただくことができ、実行委員会 として安堵するとともに、満足のいく会議であった。会議 の運営を支えてくれた秘書さん、学生の皆さんに、この場 を借りてお礼を申し上げたい。



東京大学伊藤国際学術研究センター・伊藤謝恩ホールにおける集合写真

## <u>ロ頭発表プログラム</u>

Monday, 20 November 2017

15:00	Jun Yoshinobu, Opening remarks	
15:10	Wilson Ho "Single Molecule Dynamics in Space-Time"	
15:40	Jan Patrick Dela Cruz Calupitan, "STM studies of highly-sensitive photoswitching terarylenes"	
16:00	16:00 Kana Yamagiwa, "Observation of Surface Plasmon Polaritons Propagating at the Interfaces of Organic	
	Monolayers/Au(111) by Two-Photon PEEM"	
16:20	Riku Shibuya, "Bottom-up design of N-containing carbon catalyst for oxygen reduction reaction"	
16:40	Jie Hou, "Inter-molecule interaction for magnetic property of vanadyl tetrakis(thiadiazole) porphyrazine	
	film on Au(111)"	
17:00	Manabu Kiguchi, "Site Selection of Single Molecule bridging Metal Electrodes with Surface Enhanced	
	Raman cattering"	
17:30	Welcome get-together	

Tuesday, 21 November 2017

## Water and excited processes (Chair: Ryuichi Arafune)

09:00	Yoshiyasu Matsumoto "Molecular orientations in water ice film and at its surface"
09:30	Mischa Bonn "Surface Melting and Hydrogen Bonding at the Surface of Water Ice"
10:00	Takashi Yamada "Unoccupied electronic states at the perylene/graphite interface investigated by 2PPE"
10:20	Tea break

## Water at surfaces (Chair: Yoshiyasu Matsumoto)

10:40	Miquel Salmeron "Water at interfaces - from molecules to ice and to liquid
11:10	Zdenek Dohnalek "Adsorption and Dissociation Dynamics of Water on ${\rm TiO_2}$ Surfaces: Combined
	Molecular Beam Scattering and Scanning Tunneling Microscopy Studies"
11:40	Soon Jung Jung "Engineering the TiO <sub>2</sub> Anatase (101) surface"
12:00	Lunch

## Ultrafast phenomena (Chair: Toshiaki Munakata)

13:30	Hrvoje Petek "Ultrafast electron dynamics at molecule-metal nanoparticle-semi(conductor/metal)
	heterstructures"
14:00	Hirohito Ogasawara "Elucidation of surface reaction pathway using X-ray free electron laser"
14:30	Martin Wolf "Ultrafast Excited State Dynamics and Photoinducted Phase Transitions at Interfaces"
15:00	Tea break

## Low-dimensional materials at surfaces (Chair: Noriaki Takagi)

15:30	José Ignacio Pascual "Elementary phenomena in hybrid graphene nanoribbons on surfaces"
16:00	Grant Simpson "Dipole-mediated single-molecule manipulation"
16:20	Michiko Kusunoki "Exploitation of High Quality Graphene and Novel Atomic Layers"
16:50	Shinya Yoshimoto "Gas exposure effects on monolayer pentacene field-effect transistor studied by liquid
	metal GaIn probes"
17:10	Iwao Matsuda "Novel Properties of Dirac Fermions in Borophene"

## 18:00 Poster session (Chair: Satoshi Watanabe)

Wednesday,	22	November	2017
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Catalysis (	Chair:	Katsuvuki	Fukutani)
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- 09:00 Kazunari Domen "Water splitting on particulate photocatalysts"
- 09:30 Takato Mitsudome "Cooperative Catalysis between Metal and Oxide for Environmentally Friendly Molecular Transformations"
- 10:00 Sylvain Clair "Symmetry-driven catalytic activity of silver surfaces"
- 10:20 Tea break

#### Catalysis (Chair: Zdenek Dohnalek)

- 10:40 Michael Trenary "Spectroscopic Characterization of Reaction Pathways over a Pd-Cu(111) Single-Atom Alloy"
- 11:10 Atsushi Urakawa "Hunting Surface Intermediates and Active Sites in Carbon Dioxide Conversion Catalysis"
- 11:40 Peter McBreen "Structure and Dynamics of Single Chirality-Transfer Complexes on Pt(111)"
- 12:00 Lunch

#### Functional molecules at surface and interface (Chair: Tadahiro Komeda)

- 13:30 Rasmita Raval "Supramolecular and Covalent Assembly of Molecules at Surfaces: Chirality, Complexity and Diversity"
- 14:00 Jun Terao "Synthesis of Functionalized Molecular Wires"
- 14:30 Ryo Yamada "Current Rectification of Single-Molecule Carbazole-Oligomer Junctions: the Role of Asymmetrical Deformations of Molecular Orbitals"
- 15:00 Tea break

### Single molecule spectroscopy and transport (Chair: Yousoo Kim)

- 15:30 Maki Kawai "Variety of Molecular Functions Induced by the Interaction with Substrates"
- 16:00 Jascha Repp "Tracking the ultrafast motion of a single molecule by femtosecond terahertz scanning tunneling microscopy"
- 16:30 Hiroshi Okuyama "Controlled switching of single-molecule junctions by mechanical motion of a phenyl ring"
- 17:00 Masaru Tsukada "Theoretical Aspects of SPM and Transport in Molecules"
- 17:30 **Student prize award ceremony** (Junji Nakamura)
- 19:00 **Banquet** (at Toutenko (東天紅))

#### Thursday, 23 November 2017

### Low-dimensional exotic materials (Chair: Iwao Matsuda)

- 09:00 Young Kuk "Electronic and Phononic Structure Measurements on Superconducting Surfaces using Scanning Tunneling Microscopy"
- 09:30 Mikito Koshino "Physics of Moiré Interfaces in 2D Materials"
- 10:00 Yasuo Yoshida "Direct visualization of surface-induced orbital order"
- 10:20 Tea break

### Low-dimensional materials at surfaces (Chair: Yoshitada Morikawa)

- 10:40 Nicolas Lorente "Magnetic impurities on superconducting surfaces: Shiba and Majorana states studied with the STM"
- 11:10 Emi Minamitani "Atomic-Scale Investigation of the Interfacial Phonon at Graphene/SiC"

- 11:40 Tetsuroh Shirasawa "Tracking of Solid-Liquid Interfaces by a High-Speed Surface X-ray Diffraction"
- 12:10 Lunch

### Bio-molecules and 2D materials (Chair: Tadahiro Komeda)

- 13:30 Ayumi Hirano-Iwata "Reconstitution of Ion Channel Functions in Artificially Formed Cell Membranes"
- 14:00 Takashi Kumagai "Near-Field Induced Chemistry Studied by Scanning Tunneling Microscopy"
- 14:30 Renato Zenobi "Tip-enhanced Raman Spectroscopy for Nanoscale Molecular Analysis and Imaging of 2-Dimensional Materials"
- 15:00 Ulrike Diebold "Using SPM to following single-molecule reactions on oxide surfaces"
- 15:30 Noriaki Takagi, Closing Remarks

#### Poster (student)

- PS1 Kanako Imamura "Properties of ammonia synthesis devises from water and nitrogen using electricity"
- PS2 Toshiaki Kamoshida "Chemical Characterization of Group 3-5 Transition Metal Atom-Encapsulating Si<sub>16</sub> Cage Superatoms on an Organic Surface"
- PS3 Shuya Aoyama, Jun Kaiwa "Fluctuation of charge densities during the oxygen reduction reaction process of FeN<sub>4</sub> center embedded on the carbon system"
- PS4 Ryota Osuga "Far-IR study of low frequency modes on various zeolites"
- PS5 Takafumi Higuchi "Local electronic states at picene-metal interface studied by electron spectroscopy and first-principles calculation"
- PS6 Naoki Nagatsuka "Hydrogen adsorption on and diffusion into anatase TiO2 (101) surfaces"
- PS7 Fumiaki Kato "Two competing nuclear quantum effects in hydrogen-bond breaking"
- PS8 Etty Nurlia Kusumawati "Immobilized Metal Nanoparticles Containing Ionic Liquids on SBA-15 for pnitrophenol Reduction"
- PS9 Daiki Nishiori "Photochemical Hydrogen Evolution with Cyanobacterial Photosystem I Platinum Nanoparticle Hybrid Systems"
- PS10 Yasutaka Tsuda "Surface oxide formation of copper alloys with energetic oxygen molecules"
- PS11 Hirokatsu Kurosu "Elucidating the role of phosphate and borate ions adsorbing onto cobalt oxygen evolving catalysts by in-situ observations"
- PS12 Tomoki Hiue "Enhancement of oxygen evolution activity for the cobalt oxide catalyst by coordination of glycine and its elucidation of the function"
- PS13 Raphaëll Salles "Photosystem I immobilization on PtNP nanosheet"
- PS14 Shun Fukami "Correlation Between High Gas Sensitivity and Dopant Structure in W-doped ZnO"
- PS15 Hiroki Yamamoto "Iridium clusters protected by phenylacetylene: size-controlled synthesis and structural characterization"
- PS16 Shingo Hasegawa "Emergence of Hydrogenation Catalysis in PVP-Stabilized Gold Clusters by Doping a Single Palladium Atom"
- PS17 Tsubasa Omoda "Ligand-induced transformation of gold core of [Au<sub>25</sub>(SR)<sub>18</sub>]-"
- PS18 Yuriko Tsumura "STM/STS study of stacked donor-acceptor molecules formed on Cu(111)"
- PS19 Septia Eka Marsha Putra "Formic Acid Decomposition on the Cu(111) Surface: Single Molecule and Polymeric Structure"
- PS20 Hiroki Miyazaki "The measurement of electronegativity of individual atoms using chemically defined AFM tips"
- PS21 Kohei Terasaki "STM imaging of various structures of DNA on Au(111) surface"
- PS22 Nazriq Nana "Dipole-induced interactive manipulation of single molecules"

- PS23 Kensuke Kimura "Phosphorescence detection from a single molecule with an STM"
- PS24 Hiroyuki Koshida "Formation of (NO)3 and (NO)4-water on Cu(111)"
- PS25 Youngjoon An "Interfacial electronic structures between pi-conjugated molecules on Au(111)"
- PS26 Chun Ouyang "Electron Tunnelling through Rigid Molecular Wire Anchored between Nanogap Electrodes and on Metal Surface"
- PS27 Minhui Lee "Computational study on the formation of a highly-ordered hydroxylated graphene epitaxially-grown on Cu(111)"
- PS28 Luo Uei Liang "Scanning tunneling microscope study of Phenacene Derivatives on Au(111)"
- PS29 Peiying Li "Exploration of fluorescent-tagged peptides diffusing on boron nitride by single molecular imaging"
- PS30 Natsuhiko Shimizu "High yield safe synthesis of black phosphorus"
- PS31 Takakazu Seki "Electrochemical modulation of peptides organization on two-dimensional materials"
- PS32 Fumihiro Imoto "First-principles study of the atomic and electronic structure of the 4H-SiC(1102)-(2x1) surface"
- PS33 Kohei Sakuma "Structural stability of self-assembled peptides as a molecular scaffold on 2D nanomaterials for Biosensors"
- PS34 Maria Herminia Balgos "Spatio-temporal characterization of the electrical and optical properties of LT-GaAs structures for THz applications"
- PS35 Yuhei Kikuchi "The dielectric function of atomically thin MoS<sub>2</sub>, MoSe<sub>2</sub>, WS<sub>2</sub>, and WSe<sub>2</sub> observed by linear and non-linear optical measurements"
- PS36 Shigemi Terakawa "Electronic structure and phase transition of In/Si(111)  $\sqrt{7} \times \sqrt{3}$  -hex surface"
- PS37 Yu-Hsiang Yen "Scanning tunneling microscope study of a mixed phase 2D self-assembly organic system: PTCDA on Au(111)"

#### POSTER (contributed)

- P1 Siew San Tan "Improvement of the Variation of Absorption Intensities with pH of Ruthenium(II) Polypyridine Complex with Elongation of the Conjugated Ligands: An Experimental and Theoretical Investigations"
- P2 Shuhei Ogo "Reaction mechanisms of oxidative coupling of methane over Ce<sub>2</sub>(WO<sub>4</sub>)<sub>3</sub> catalysts at low temperatures in an electric field"
- P3 Akira Yamakata "Principal Difference in the Behaviors of Photogenerated e- and h+ in Anatase and Rutile TiO<sub>2</sub> Powders"
- P4 Taketoshi Minato "Interface Structure between Graphite and Organic Electrolyte Investigated by Frequency Modulation Atomic Force Microscopy"
- P5 Takanori Koitaya "Activation of carbon dioxide on Zn-deposited Cu surfaces studied by ambient-pressure X-ray photoelectron spectroscopy"
- P6 Shen Ye "Structure and Stability of the Lipid Monolayer on the Water Surface"
- P7 Susumu Shiraki "Very-Low Solid-Electrolyte/Electrode Interface Resistance in Li(Ni<sub>0.5</sub>Mn<sub>1.5</sub>)O<sub>4</sub>-Based Thin-Film Battery"
- P8 Canceled
- P9 Kenichi Ozawa "Carrier lifetime as a primary factor for crystal-face dependence of photocatalytic activity on rutile and anatase TiO<sub>2</sub>"
- P10 Fahdzi Muttaqien "Dynamics of Desorbed CO2 as a Product of Formate Decomposition"
- P11 Ingo Salzmann "Local processes in the molecular doping of poly(3-hexylthiophene)"
- P12 Qiuyi Yuan "Reaction mechanism of Galvanic Displacement Reaction of Pt on Au(111)"

- P13 Akira Nakayama "Catalytic Reactions at the Water/CeO<sub>2</sub> Interface: Hydration of 2-Cyanopyridine"
- P14 Francesca Celine Catalan "Facet-dependent anodic corrosion in boron-doped diamond electrode surface"
- P15 Jiamei Quan "Bending-mode induced CO<sub>2</sub> hydrogenation on Cu catalysts via Eley-Rideal type mechanism"
- P16 Hiroyuki S. Kato "Predesigned Formation of Strongly Hydrogen-Bonding Heterogeneous Bilayer on Au(111)"
- P17 Kosuke Yamazoe "Hydrogen-bonding network of water in a charged polymer brush"
- P18 Nobuyuki Fukui "Geometry control of size selected Pt cluster supported on substrate by cluster impact deposition"
- P19 Takehiko Sasaki "Functionalized Graphene Oxide for Catalytic Reactions"
- P20 Lay Thithi "Surface and Interfacial Reaction of Al<sub>2</sub>O<sub>3</sub>/SiO<sub>2</sub>/Si films by SR-XPS"
- P21 Yoshihisa Harada "Single atom, 2D, 3D distributed Pt atoms on graphene sheets studied by in situ X-Ray absorption fine structures and theoretical simulation"
- P22 Yoshihisa Harada "Probing the OH Stretch in Different Local Environments In Liquid Water"
- P23 Hisato Yasumatsu "Low-temperature catalytic activity driven by uni-sized Pt clusters bound to Si surface in CO oxidation and NO reduction"
- P24 Hironobu Hayashi "On-surface Formation of Au-Directed Heptacene Organometallic Complexes on a Au(111)
  Template"
- P25 Susumu Yamamoto "Adsorption and reaction of CO2 on graphene studied by ambient pressure XPS"
- P26 Kenta Motobayashi "Interfacial Structures of Ionic Liquids Affecting Electrochemical Reactions: A Surface-Enhanced Infrared Study"
- P27 Koichiro Yamakawa "Significantly enhanced infrared absorption by CO<sub>2</sub> adsorbed on clean and defected surfaces of anatase TiO<sub>2</sub>(101)"
- P28 Jongsik Kim "MIL-47 (V)-Derived, V Leaching-Resistant V Carbide on Carbon Catalyst for Oxidative Desulfurization of Aromatic Sulfur"
- P29 Kazuo Watanabe "Photoreactions of  $\mathrm{O}_2$  on undulated Pd(111) surfaces"
- P30 Tatsuhiko Ohto "Trimethylamine-N-oxide: its hydration structure and surface activity, viewed by vibrational spectroscopy and molecular dynamics simulations"
- P31 Nan Jiang "An Insight into Single-Molecule Chemistry via Scanning Tunneling Microscopy Imaging and Advanced Raman Spectroscopy Techniques"
- P32 Aran Garcia-Lekue "Electron Transport Along a Freestanding Conjugated Molecule"
- P33 Yoshiaki Sugimoto "The nature of the chemical bond verified by noncontact AFM "
- P34 Akitoshi Shiotari "Ultrahigh-resolution imaging of water networks on Cu(110) by atomic force microscopy"
- P35 Masayuki Hamada "The measurement of the surface conductivity on the Si(111)-7x7 surface by scanning tunneling potentiometry"
- P36 Yasuyuki Yokota "Development of Tip-Enhanced Raman Spectroscopy for Electrochemical Interfaces"
- P37 Tomoko Shimizu "Simultaneous STM/AFM measurement of meso-dibenzoporphycene"
- P38 Emiko Kazuma "Visible-light-induced molecular photodissociation on metal surfaces"
- P39 Toshiki Sugimoto "Inelastic Electron Tunneling Mediated by Molecular Quantum Rotator"
- P40 Kuniyuki Miwa "Interference effects on scanning tunneling microscope-induced light emission from coupled system of molecular exciton and interface plasmons"
- P41 Hyung-Joon Shin "Real-space imaging of multiple electron scatterings in a single graphene"
- P42 Shunji Yamamoto "Direct Visualization of Surface Phase of Oxygen Molecules Physisorbed on the Ag(111) Surface: A Two-dimensional Quantum Spin System"

- P43 Eiichi Inami "Room temperature stable film formation of  $\pi$ -conjugated organic molecules on 3d-magnetic substrate"
- P44 Songpol Chaunchaiyakul "Nanoscale Dehydrogenation on a Self-Assembled Monolayer Observed by Tip-Enhanced Raman Spectroscopy"
- P45 Holly Walen "Sulfur atom adsorption on Cu surfaces: Characterization and Stability"
- P46 Norio Okabayashi "Vibrational state of a single molecule influenced by the force from a tip"
- P47 Kozo Mukai "Electronic states of Pt single atom and cluster supported on graphene studied by synchrotron radiation XPS"
- P48 Puneet Mishra "Spatially Resolved Magnetic Anisotropy of Cobalt Nanostructures on Au(111) Surface"
- P49 Rafael Jaculbia "Towards single molecule nanospectroscopy in LT-UHV environment using STM-TERS"
- P50 Shiro Yamazaki "AFM/STM-induced atom-scale catalytic switching of molecule-like Si "
- P51 Hiroshi Imada "Single-molecule investigation of plasmon-exciton coupling"
- P52 Ryuichi Arafune "Spectroscopic demonstration of surface opto-spincurrent on Ir(111) covered by graphene"
- P53 Shin-ichiro Tanaka "Direct observation of the electron-phonon coupling between empty states in graphite via high-resolution electron energy loss spectroscopy"
- P54 Zheng Liu "In-Situ Observation of H-BN/Graphene Heterostructure Synthesized in a STEM"
- P55 Chun-Liang Lin "Quasiparticle Scattering in Type-II Weyl semimetal MoTe<sub>2</sub>"
- P56 Masahiro Shibuta "Observation of Two-Dimensionally Delocalized Exciton Confined in an Aromatic Molecular Monolayer Formed on Organic Insulating Layer"
- P57 Hung-Hsiang Yang "Protecting Topological Surface State by Organic Monolayer"
- P58 Shozo Suto "Preparation of the anisotropic low dimensional structure of hydrogen terminated Si(110)-(1x1) surface: Structures, electronic band structures, surface phonons and applications"
- P59 Md. Zakir Hossain "Solution processed organic functionalization of graphene"
- P60 Takahiro Kondo "Hydrogen boride sheets derived from MgB2 by cation exchange"
- P61 Matthias Koch "Single shot spin readout with a 3D crystalline transistor"
- P62 Zeyuan Ni "Germanene and stanene on 2D substrates: Dirac-cone and Z2 invariant"
- P63 Chi-Cheng Lee "Studies of absolute binding energies of core electrons in epitaxial silicene on ZrB2(0001)"
- P64 Fumio Komori "Graphene nanoribbons on periodic nanofacets of SiC"
- P65 Shohei Ogura "Development of a spin-polarized atomic hydrogen beam"
- P66 Jun Yoshinobu "Oxidation and nitridation of silicene on ZrB<sub>2</sub>/Si(111) with NO"
- P67 Hiroko Yamada "On-Surface Reactivity Investigation of Partially Fluorinated Anthracene Trimers on Au(111)"

なお、本国際会議の要旨集は以下の URL からダウンロードすることができる。

http://yoshinobu.issp.u-tokyo.ac.jp/ IIRC5\_Program\_booklet-Final.pdf