

The 6th Japan-Sweden Workshop

on

**Advanced Spectroscopy of
Organic Materials for Electronic Applications**

ASOMEA-VI

Wednesday 23 - Saturday 26 November 2011

Kaga-Onsen, Ishikawa, Japan

THE ORGANIZING COMMITTEE

Rainer Friedlein, JAIST, Japan

Yoshitada Morikawa, Osaka University, Japan

Hiroyuki Yoshida, Kyoto University, Japan

Mats Fahlman, Linköping University, Sweden

Richard Murdey, Kyoto University, Japan

Tomoya Ono, Osaka University, Japan

Hidekazu Goto, Osaka University, Japan

Kouji Inagaki, Osaka University, Japan

William R. Salaneck, Linköping University, Sweden

Nobuo Ueno, Global-COE, Chiba University, Japan

SPONSORS

Chiba COE

JAIST, School of Materials Science

Kaga City

VG Scienta

ADCAP Vacuum Technologies Co., Ltd

Bunkohkeiki Co., Ltd.

Ailin Vacuum Co., Ltd

Gen-Tech, Inc.

WORKSHOP SCHEDULE

NOVEMBER 23 WEDNESDAY	NOVEMBER 24 THURSDAY	NOVEMBER 25 FRIDAY	NOVEMBER 26 SATURDAY
	Opening remarks 8:45 – 9:00		
	Session 1 9:00 – 10:50	Session 4 9:00 – 10:50	Session 8 9:00 – 10:50
	Coffee break 10:50 – 11:10		
	Session 2 11:10 – 12:30	Session 5 11:10 – 12:30	Session 9 11:10 – 12:30
	Lunch 12:30 – 14:00	(Photo)	Lunch 12:30 – 13:30
	Session 3 14:00 – 16:00	Session 6 14:00 – 15:30	Session 10 13:30 – 15:00
			Closing remarks 15:00 – 15:10
Registration 15:00 – 17:00 (Lobby)		Coffee break 15:30 – 15:50	
	Poster session 16:00 – 17:30	Session 7 15:50 – 17:20	
Mixer 17:00 – 20:00 (Banquet Hall)		Break	
	Dinner (Restaurant)	Banquet 18:30 – 20:00 (Banquet Hall)	

THURSDAY, NOVEMBER 24

8:45 – 9:50 *opening remarks by Rainer Friedlein*

8:50 – 9:00 *introductory remarks by William R. Salaneck*

9:00 – 10:50 AM	Session 1	Nobuo Ueno, chair
9:00	Charge transfer and polarization at interfaces with conjugated molecules (1-1S) <i>Norbert Koch</i>	
9:50	Electronic structures of novel metal-on-organic and organic-on-metal interfaces (1-2A) <i>Yasuo Nakayama</i>	
10:20	Role of the van der Waals interaction at organic/metal interfaces: energetics, adsorption geometry, and energy level alignment (1-3A) <i>Susumu Yanagisawa</i>	

11:50 – 11:10 coffee break

11:10 – 12:30	Session 2	Takashi Fujikawa, chair
11:10	Studies of nanostructured films by means of electron spectroscopy (2-1A) <i>Hans Siegbahn</i>	
11:40	Electrolyte-gated organic field-effect transistors (2-2A) <i>Xavier Crispin</i>	
12:10	Effect of oxygen on the electronic structure of highly-crystalline picene films (2-3L) <i>Ying Wang</i>	

12:30 – 14:00 lunch

14:00 – 16:00	Session 3	Toshiaki Munakata, chair
14:00	Thin film pentacene on the chemically modified Si(100) surfaces: growth, energy level alignment and electronic states (3-1A) <i>Jun Yoshinobu</i>	
14:30	Theory of photoemission from organic solids (3-2A) <i>Takashi Fujikawa</i>	
15:00	Core-energy level difference in the surface and bulk regions of organic semiconductor films studied by X-ray photoemission spectroscopy with depth resolution (3-3A) <i>Hiroyuki Yoshida</i>	
15:30	A new multidimensional electron spectrometer: Impact on molecular electronics research (3-4A) <i>Antje Vollmer</i>	

16:00 – 17:30 poster session

16:00 – 17:30	Poster Session
P-1	First-principles study on spin-polarized electric current in C/BN hetero-nanotubes <i>Nguyen Duy Huy</i>
P-2	Electron-electron correlation energy calculations by superposition of non-orthogonal Slater determinants <i>Akira Sasaki</i>
P-3	Desorption behaviors of alkanethiol self-assembled monolayers studied by thermal desorption spectroscopy <i>Eisuke Ito</i>
P-4	Giant surface potential due to spontaneous noncentrosymmetric molecular orientation in vacuum-deposited thin film of Alq ₃ derivatives <i>Takashi Isoshima</i>
P-5	Correlation between energy level alignment and device performance in small-molecule based organic photovoltaic cells <i>Kouki Akaike</i>
P-6	Study on the electronic properties of C ₆₀ and bathocuproine interface using ultraviolet photoelectron spectroscopy <i>Shenghao Wang</i>
P-7	Characterization of an organic thin film device under operational condition by fluorescence-yield X-ray absorption spectroscopy <i>Hiroyuki S. Kato</i>
P-8	Local and global electronic spectroscopy of unoccupied states: Naphthalene on HOPG studied by the combination of 2PPE and STM <i>Takashi Yamada</i>
P-9	Experimental study of epitaxial silicene on zirconium diboride <i>Antoine Fleurence</i>
P-10	van der Waals density functional applied to adsorption systems <i>Ikutaro Hamada</i>
P-11	First-principles study of CO oxidation on carbon alloy catalysts <i>Shintaro Iseki</i>

FRIDAY, NOVEMBER 25

9:00 – 10:50	Session 4	Hans Siegbahn, chair
9:00	Interaction at hetero-epitaxial organic interfaces: Phthalocyanine and PTCDA molecules on noble metal surfaces (4-1S) <i>Christian Kumpf</i>	
9:50	Theoretical study of dipole layer formation at organic/metal interfaces (4-2A) <i>Yoshitada Morikawa</i>	
10:20	Giant surface potential due to spontaneous noncentrosymmetric molecular orientation in vacuum-deposited thin film of Alq ₃ derivatives (4-3A) <i>Takashi Isoshima</i>	

11:50-11:10 coffee break

11:10 – 12:30	Session 5	Jun Yoshinobu, chair
11:10	Organic and hybrid organic heterojunctions in organic electronics and spintronics applications (5-1A) <i>Mats Fahlman</i>	
11:40	Electronic structure of a cobalt-phthalocyanine adsorbed quasi-one dimensional Ag surface (5-2A) <i>Kazuyuki Sakamoto</i>	
12:10	Theoretical proposal for indirect measurement of weakly-coupled adsorbates on quasi-1D metallic substrate by STS (5-3L) <i>Masayuki Yamamoto</i>	

12:30 – 12:40 photo

12:40 – 14:00 lunch

14:00 – 15:30	Session 6	Hiroyuki Yamane, chair
14:00	Electronic excitation of rubrene/HOPG mediated by image potential state (6-1A) <i>Toshiaki Munakata</i>	
14:30	Development of the HELIOS laboratory for time-resolved VUV/soft X-ray pump-probe studies at Uppsala University, Sweden (6-2A) <i>Johan Söderström</i>	
15:00	The photoconductivity of pentacene thin films as a function of thickness (6-3A) <i>Richard Murdey</i>	

15:30 – 15:50 coffee break

15:50 – 17:20	Session 7	Xavier Crispin, chair
15:50	Spin-polarized current through graphene nanoflake (7-1A) <i>Tomoya Ono</i>	
16:20	Interfacial electronic properties between organic semiconductor and graphene films (7-2A) <i>Xianjie Liu</i>	
16:50	Structural and electronic properties of epitaxial silicene (7-3A) <i>Yukiko Yamada-Takamura</i>	

SATURDAY, NOVEMBER 26

9:00 – 10:50	Session 8	Hisao Ishii, chair
9:00	Charge transport in organic semiconductors: A theoretical perspective (8-1S) <i>Veaceslav Coropceanu</i>	
9:50	Insight into the HOMO hole in π -conjugated molecules as dielectric medium (8-2A) <i>Satoshi Kera</i>	
10:20	Charge reorganization energy and small polaron binding energy of rubrene thin films by UPS (8-3A) <i>Steffen Duhm</i>	

11:50 – 11:10 coffee break

11:10 – 12:30	Session 9	Satoshi Kera, chair
11:10	Multi-scale transport calculations for nanomaterial systems (9-1A) <i>Kenji Hirose</i>	
11:40	Intermolecular interaction in crystalline films of phthalocyanines probed by high-resolution photoelectron spectroscopy (9-2A) <i>Hiroyuki Yamane</i>	
12:10	Pentacene thin film on SiO ₂ substrate: Electronic properties vs. growth conditions (9-3L) <i>Fabio Bussolotti</i>	

12:30 – 13:30 lunch

13:30 – 15:00	Session 10	Mats Fahlman, chair
13:30	Extended electronic states in self-assembled genetic matter (10-1A) <i>Rainer Friedlein</i>	
14:00	Fabrication of highly ordered organic biradical molecular film (10-2A) <i>Kaname Kanai</i>	
14:30	Electronic structures of organic semiconductors studied by photoelectron yield spectroscopy: From single crystal to liquid sample (10-3A) <i>Hisao Ishii</i>	

15:00 – 15:10 closing remarks by Yoshitada Morikawa

ABSTRACTS FOR ORAL PRESENTATIONS

Charge transfer and polarization at interfaces with conjugated molecules

Johannes Frisch¹, Patrick Amsalem¹, Jens Niederhausen¹, Antje Vollmer², Norbert Koch¹

¹*Humboldt-Universität zu Berlin, Institut für Physik, Newtonstr. 15, 12489 Berlin, Germany*

²*Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, BESSY II, Albert-Einstein-Str. 15, 12489 Berlin, Germany*

E-mail: norbert.koch@physik.hu-berlin.de

The function and efficiency of organic electronic devices is determined to a significant extent by the electronic properties of organic/organic heterojunctions and interfaces between electrodes and organic semiconductors. The energy level alignment between metal electrodes and active organic layers can be adjusted over wide ranges by employing interlayers of strong molecular acceptors and donors that undergo charge transfer reactions with the metal. It will be shown that such interlayers lead to lower charge injection barriers than pristine metals, even when the work function is the same [1]. It is argued that the molecularly modified electrodes are electronically more rigid than their pristine metal counterparts, i.e., the electron spill-out at the organic-terminated surface is less pronounced compared to metal surfaces [2].

The energy levels at organic/organic heterojunctions comprising donors and acceptors as used in organic photovoltaic cells are essentially independent of deposition sequence, as long as supporting electrodes do not induce energy level pinning. When a high work function electrode is used, the energy levels may become Fermi-level pinned and an electric field drops right at the heterojunction. This effect is exemplified for the donor diindenoperylene and the acceptor C₆₀ [3]. The electric field distribution within an organic opto-electronic device may thus be adjusted locally by employing interfacial energy level pinning, even at weakly interacting organic/organic interfaces.

References

[1] B. Bröker, et al., *Phys. Rev. Lett.* 104 (2010) 246805.

[2] J. Niederhausen, P. Amsalem, J. Frisch, A. Wilke, A. Vollmer, R. Rieger, K. Müllen, J. P. Rabe, N. Koch, *Phys. Rev. B* 84 (2011) 165302.

[3] A. Wilke, P. Amsalem, J. Frisch, B. Bröker, A. Vollmer, N. Koch, *Appl. Phys. Lett.* 98 (2011) 123304.

1-2A

Electronic structures of novel metal-on-organic and organic-on-metal interfaces

Y. Nakayama¹, S. Machida², J. Niederhausen³, H. Kinjo², C.-H. Chen⁴, C.-C. Hsu⁴, M.-K. Lin⁴, C.-Y. Wang⁴, A. Vollmer⁵, T.-W. Pi⁶, S.-J. Tang^{4,6}, N. Koch³, H. Ishii^{1,3}

¹Center for Frontier Science, Chiba University, Japan

²Graduate School of Advanced Integration Science, Chiba University, Japan

³Department of Physics, Humboldt-University of Berlin, Germany

⁴Department of Physics and Astronomy, National Tsing-Hua University, Taiwan

⁵Helmholtz Zentrum Berlin für Materialien und Energie GmbH Elektronenspeicherring BESSY II, Germany

⁶National Synchrotron Radiation Research Center (NSRRC), Taiwan

E-mail: nkym@restaff.chiba-u.jp

The electronic structure of interfaces between metals and organic materials plays a crucial role for the performance of the organic electronics devices. Extensive studies by photoelectron spectroscopy on well-defined interfaces of organic thin layers on metal single crystal surfaces have so far provided useful information to guide the realization of metal-organic junctions for improved practical devices [1]. We are now attempting to extend the matured metal-organic “surface science” toward two types of frontier interfaces, metal on organic single crystal surfaces and organic molecules on two-dimensionally quantized metal surfaces, by means of angle-resolved photoelectron spectroscopy (ARPES). A technical challenge, suppressing sample charging caused by insufficient compensation of emitted photoelectrons, had to be overcome to endeavor the former target. We primarily succeeded to determine the highest occupied molecular orbital (HOMO) energy of a rubrene single crystal by photoelectron yield spectroscopy (PYS) [2], and to evaluate the hole effective mass of the HOMO-derived band through ARPES measurement assisted by laser-light illumination [3]. Also employing these techniques, we have studied the electronic structures of rubrene single crystals covered with metals. For the latter topic, a novel interface electronic structure of phthalocyanine molecules and “quantum well states” that are generated in a few nanometer thin metal films formed on (inorganic) semiconductor substrates will also be presented.

References

- [1] *e.g.* N. Ueno, S. Kera, *Prog. Surf. Sci.* **83**, 490 (2008).
- [2] Y. Nakayama, *et al.*, *Appl. Phys. Lett.* **92**, 153306 (2008); *ibid.*, **93**, 173305 (2008).
- [3] S. Machida, *et al.*, *Phys. Rev. Lett.* **104**, 156401 (2010).

Role of the van der Waals interaction at organic/metal interfaces: energetics, adsorption geometry, and energy level alignment

Susumu Yanagisawa¹, Takahiro Saigo², and Yoshitada Morikawa²

¹*Department of Physics and Earth Sciences, University of the Ryukyus, 1 Senbaru, Nishihara, Okinawa, 903-0213, Japan*

²*Department of Precision Science and Technology, Graduate School of Engineering, Osaka University, 2-1 Yamada-oka, Suita, Osaka 565-0871, Japan*

E-mail: shou@phys.u-ryukyu.ac.jp

An electric dipole layer at an organic/metal interface significantly alters the energy level alignment between the organic layer and the metal electrode, and thus determines a carrier injection barrier [1]. Our first-principles theoretical study clarified that the interface geometry, especially, the organic-metal distance is an important factor determining the interface dipole [2,3]. Therefore, it is of critical importance to calculate atomic geometries at organic/metal interfaces accurately to predict interface dipoles and to design interfaces with appropriate electronic properties. We demonstrated that density functional theory (DFT) with recently proposed van der Waals (vdW) corrections [4,5] accurately reproduces organic/metal interface geometries and interface dipoles [3,6].

In this talk, we will demonstrate our recent progress in understanding the nature of the interaction at organic/metal interfaces. First, we describe the subtle interplay between covalent bonds, vdW attraction, and structural distortion in the chemisorption of tris-(8-hydroxyquinoline) aluminum (Alq₃) on metal surfaces [6]. Next, based on the accurate adsorption geometries obtained with the vdW correction method, we propose a novel way to control the interface level alignment by applying mechanical stress at the carbon nanotube (CNT)/metal interface, with which both *p*-type and *n*-type channels can be formed using Au as electrodes [7].

References

- [1] H. Ishii, H. Ishii, K. Sugiyama, E. Ito, and K. Seki, *Adv. Mater.* **11**, 605 (1999).
- [2] Y. Morikawa, H. Ishii, and K. Seki, *Phys. Rev. B* **69**, 041403(R) (2004).
- [3] K. Toyoda, I. Hamada, K. Lee, S. Yanagisawa, and Y. Morikawa, *J. Chem. Phys.* **132**, 134703 (2010).
- [4] S. Grimme, *J. Comput. Chem.* **27**, 1787 (2006).
- [5] M. Dion, H. Rydberg, E. Schröder, D. C. Langreth, and B. I. Lundqvist, *Phys. Rev. Lett.* **92**, 246401 (2004).
- [6] S. Yanagisawa, I. Hamada, K. Lee, D. C. Langreth, and Y. Morikawa, *Phys. Rev. B* **83**, 235412 (2011).
- [7] T. Saigo, S. Yanagisawa, and Y. Morikawa, *in preparation*.

2-1A

Studies of nanostructured films by means of electron spectroscopy

E. M. J. Johansson¹, M. Hahlin², S. Plogmaker³, H. Rensmo³ and H. Siegbahn³

¹*Department of Physical and Analytical Chemistry, Uppsala University, Box 259, S75125 Uppsala Sweden*

²*Department of Materials Chemistry, Uppsala University, Box 538, S75121 Uppsala Sweden*

³*Department of Physics and Astronomy, Uppsala University, Box 516, S75120 Uppsala, Sweden*

Email: hans.siegbahn@fysik.uu.se

Research and development of nanostructured metal oxide films have during the last few years become an area of wide interest. This is very much related to the potential applications of such films, applications that span from electrode materials in dye-sensitized solar cells (DSC) [1], batteries and displays to photocatalysis in the gas phase or in liquids. From a morphological point of view the typical film is best viewed as a sponge, allowing a liquid medium to penetrate the solid semiconducting film all the way to the substrate. The semiconductor particles can be made transparent and can be modified by molecules anchored to the surface. The success in the use of future advanced nanostructured materials strongly depends on the detailed understanding and the possibility to control the structure-function relationship within surfaces and interfaces. Our efforts during recent years have been directed towards studies of interfaces with respect to their electrochemical function and charge transfer dynamics at a molecular level. Detailed knowledge of the properties and processes at the key interfaces is highly important to understand the relevant factors to further develop the various applications [2-5].

The present contribution reports recent results of PES and XAS, extending to the HAXPES regime, on nanostructured films and related model systems. It is shown that information may be obtained both on structural and electronic properties, which provide further understanding of the function of such films in actual devices.

References

- [1] B. O'Regan and M. Grätzel, *Nature* **353**, 737 (1991).
- [2] K. R. J. Thomas, J. T. Lin, Y. C. Hsu, and K. C. Ho, *Chem. Comm.* **32**, 4098 (2005).
- [3] D. P. Hagberg, T. Edvinsson, T. Marinado, A. H. G. Boschloo and L. Sun, *Chem. Comm.* **21**, 2245 (2006).
- [4] E. M. J. Johansson, T. Edvinsson, M. Odelius, D. P. Hagberg, L. C. Sun, A. Hagfeldt, H. Siegbahn, and H. Rensmo, *J. Phys. Chem.* **C111**, 8580 (2007).
- [5] M. Hahlin, E. M. J. Johansson, S. Plogmaker, M. Odelius, D. P. Hagberg, L. C. Sun, H. Siegbahn and H. Rensmo, *Phys. Chem. Chem. Phys.* **12**, 1507 (2010).

Electrolyte-gated organic field-effect transistors

Xavier Crispin, Ari Laiho, Oscar Larsson, Lars Herlogsson, Magnus Berggren

*Department of Science and Technology, Organic Electronics
Linköping University
SE-601 74, Norrköping (Sweden)
E-mail: xavier.crispin@liu.se*

The combination of electrolytes and organic semiconductors has opened up new opportunities in photonics, electronics and in energy storage. In most of these devices, the key mechanisms involve the transport of charge carriers (electrons or ions) across the organic semiconductor-electrolyte interface. The formation of an electric double layer (EDL) at this polarized interface is fuzzier than at a metal-electrolyte interface since weak intermolecular interactions in the organic solid favour the penetration of ions. An EDL established at the organic semiconductor-electrolyte interface, defined by a sheet of electronic charge carriers and a sheet of ions, has been proposed recently as the basic mechanism for electrolyte-gated organic field-effect transistors (EGOFETs). Here, we investigate the impact of the gate capacitance and the chemical nature of the semiconductor. We are able to distinguish clearly two regimes: (i) the “field effect” regime with a two-dimensional electronic charge carrier transport confined in the EDL located at the organic semiconductor-electrolyte interface; and, (ii) the “electrochemical” regime characterized by a three-dimensional transport in the semiconducting channel. We further develop p- and n-channel transistors and integrate those in low voltage, low power CMOS circuits.

References

- [1] Oscar Larsson, Ari Laiho, Wolfgang Schmickler, Magnus Berggren and Xavier Crispin, *Advanced Materials*, accepted.
- [2] A. Laiho, L. Herlogsson, R. Forchheimer, X. Crispin and M. Berggren, *Proceedings of the National Academy of Sciences*, online (2011)[DOI: 10.1073/pnas.1107063108].
- [3] L. Herlogsson, X. Crispin, S. Tierney, M. Berggren, *Advanced Materials*, on line (2011) [DOI: 10.1002/adma.201101757].

2-3L

Effect of oxygen on the electronic structure of highly-crystalline picene films

Ying Wang¹, Simone Di Motta², Fabrizia Negri², Rainer Friedlein¹

¹*School of Materials Science, Japan Advanced Institute of Science and Technology, 1-1 Asahidai, Nomi, Ishikawa 923-1292, Japan,*

²*Università degli Studi di Bologna, Dipartimento di Chimica "G. Ciamician", Via F. Selmi, 2 and INSTM, UdR Bologna, I - 40126 Bologna, Italy*

E-mail: wang-y@jaist.ac.jp

The underlying fundamental mechanisms of the electrical changes of organic semiconductors caused by the oxygen-*p*-doping are only partially understood so far. Recently, the performance of organic thin film transistors based on picene can be enhanced up to 5 cm²/Vs upon exposure to O₂ gas at 500 Torr.¹ This unique property of picene inspired us to study the changes of electronic structure induced by the interaction between oxygen and picene. Here, the electronic structure of highly-crystalline picene films with standing-up orientation grown epitaxially on the Ag(110) surface was investigated by angular resolved ultraviolet photoelectron spectroscopy.² Upon exposure to oxygen gas, O₂ molecules incorporate at the interstitial sites within the *a-b* plane of the film. Features related to the highest three occupied molecular orbitals shift towards lower binding energy which results in the inactivation of traps and the reduction of the charge injection barrier by about 1 eV. The original highest two picene orbitals are inverted due to the strong interactions between the singly occupied oxygen π orbital and the highest occupied orbitals of picene.

References

[1] H. Okamoto, N. Kawasaki, Y. Kaji, Y. Kubozono, A. Fujiwara, M. Yamaji, *J. Am. Chem. Soc.* **130**, 10470-10471 (2008).

[2] Y. Wang, S. D. Motta, F. KNegri, R. Friedlein, *J. Am. Chem. Soc.* **133**, 10054-10057 (2011).

Thin film pentacene on the chemically modified Si(100) surfaces: growth, energy level alignment and electronic states

J. Yoshinobu¹, K. Kameshima¹, K. Mukai¹ and S. Yoshimoto¹

¹ISSP, The University of Tokyo, Kashiwa, Chiba 277-8581 JAPAN
E-mail: yoshinobu@issp.u-tokyo.ac.jp

We prepared the ethylene terminated Si(100) (2x1) surface [1] as a chemically inert well-defined substrate for thin film growth of pentacene. In addition, a submonolayer F4-TCNQ molecules [2] were deposited on the ethylene terminated Si(100) surface in order to decrease the hole injection barrier. The electronic states were investigated *in-situ* by photoelectron spectroscopy (UPS and XPS) and the morphology of pentacene thin film was observed by *ex-situ* AFM. Fig. 1 shows an AFM image of pentacene thin film grown on the F4-TCNQ/ethylene/Si(100) surface at 300 K. Dendritic growth of pentacene with several μm domains was observed [3]. Figure 2 summarizes the energy diagram of pentacene films on the ethylene/Si(100) surface (left) and the F4-TCNQ/ethylene/Si(100) surface (right). By a submonolayer amount of F4-TCNQ deposition, the workfunction was increased by 0.97 eV, and as a result the hole injection barrier was successfully decreased from 0.98 eV to 0.47 eV.

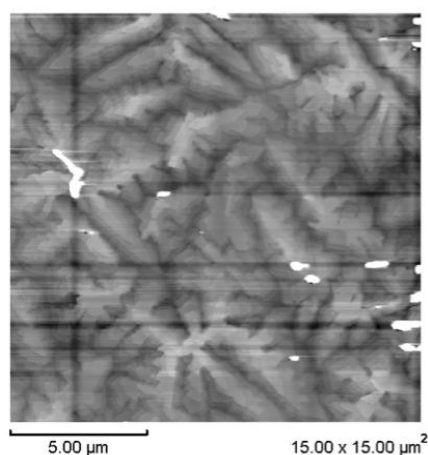


Fig. 1

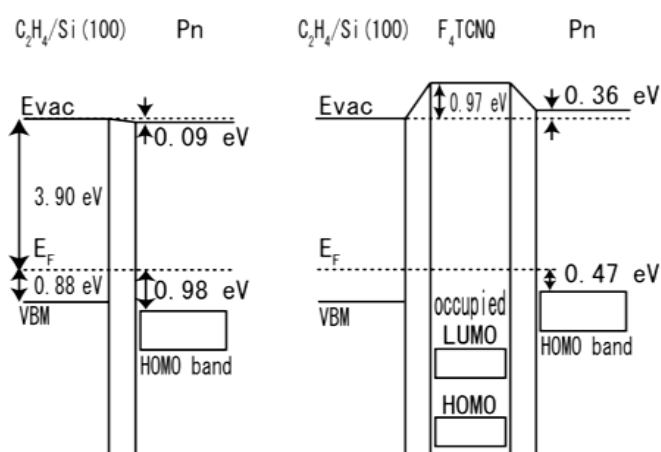


Fig. 2

References

- [1] J. Yoshinobu, H. Tsuda, M. Onchi, and M. Nishijima, *J. Chem. Phys.*, **87**, 7332-7340 (1987).
- [2] N. Koch, S. Duhm, J. P. Rabe, A. Vollmer, and R. L. Johnson, *Phys. Rev. Lett.* **95**, 237601 (2005).
- [3] H. Yanagisawa, T. Tamaki, M. Nakamura, and K. Kudo, *Thin Solid Film* **464**, 398 (2004).

3-2A

Theory of photoemission from organic solids

Takashi Fujikawa

¹Graduate School of Advanced Integration Science, Chiba University, JAPAN
E-mail: tfujikawa@faculty.chiba-u.jp

A new many-body theory of photoemission from organic solids has been developed on the basis of GW ladder approximation, that is, T-matrix approximation. In organic solids, inter-molecular interaction is weak and long-range, which is dominated by screened Coulomb interaction W . In contrast the short-range electron interaction inside the same molecule should be taken into account for the photoemission processes. This interaction is conveniently described in terms of the T-matrix (ladder) approximation expanded with screened Coulomb interaction W instead of bare Coulomb interaction v , and renormalized G ; the lowest order term is well known GW approximation. The exchange term starts from the first order, whereas the direct term starts from the third order in W . If we replace the GW term with the exchange term, both the direct and the exchange selfenergy starts from the second order terms in W . Based on the Keldysh Green's function formula [1], we calculate the hole Green's function whose electron selfenergy has both effects from W and T . Photoelectron Dyson function is influenced by the electron selfenergy: For the calculation of them, we can apply the conventional site T-matrix expansion. Further many-body corrections, radiation field screening, should be taken into account to describe the resonant behavior when ω (photon energy) is close to the plasmon energy [2].

References

- [1] T. Fujikawa and H. Arai, J. Elect. Spect. Relat. Phenom. 123 (2002) 19-46.
- [2] T. Fujikawa and H. Arai, J. Elect. Spect. Relat. Phenom. 149 (2005) 61-86.

Core-energy level difference in the surface and bulk regions of organic semiconductor films studied by X-ray photoemission spectroscopy with depth resolution

Hiroyuki Yoshida^{1,2}, Eisuke Ito³, Masahiko Hara³, Naoki Sato¹

¹Institute for Chemical Research, Kyoto University, Uji, Kyoto 611-0011, Japan

²JST, PRESTO, 4-1-8 Honcho Kawaguchi, Saitama 3312-0012, Japan

³Flucto-Order Functions Research Team, RIKEN-ASI, 2-1 Hirosawa, Wako, Saitama 351-0198 Japan

E-mail: yoshida@e.kuicr.kyoto-u.ac.jp

There has been an argument whether the energy level determined by PES is difference between the surface and bulk regions for decades. The reason was that PES is surface sensitive analysis and no appropriate experimental method has been available to distinguish the energy levels between the surface and bulk of materials.

We have recently developed a novel analytical method of the core level energies with depth resolution; X-ray photoemission spectra (XPS) are measured at multiple detection angles and the energy profiles are precisely analyzed using target factor analysis [1]. This method was applied to organic semiconductor thin films to examine the difference in core-energy levels between the surface and bulk leading to precise determination of the energy differences as well as the thickness of the surface layer.

The results show that the core-levels of the first surface layer are different from those of the bulk by an amount ranging from 0.2 to 0.4 eV. The possible origins are (a) the electrostatic polarization, (b) the surface dipole layer, and (c) preferential orientation of polar molecules as schematically shown in Figure 1. In this study, the origin is discussed from the systematical study on different organic materials [2].

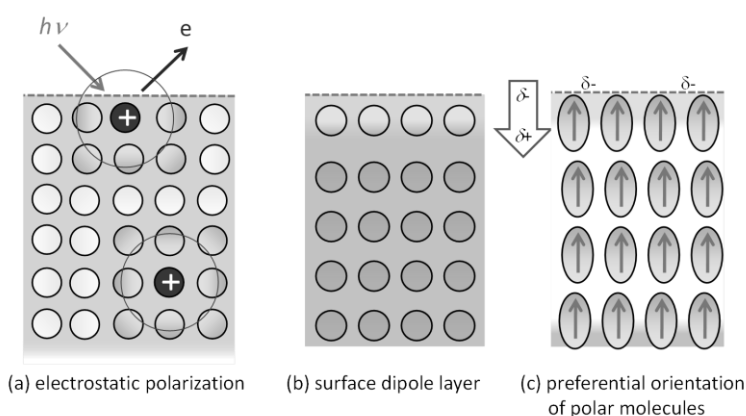


Fig 1: Possible origins of difference in the surface/bulk level energies.

References

[1] H. Yoshida, N. Sato, *Chem. Phys. Lett.*, **511**, 146 (2011).

[2] H. Yoshida, E. Ito, M. Hara, N. Sato, *Synth. Met.* (doi:10.1016/j.synthmet.2011.09.015).

3-4A

A new multidimensional electron spectrometer: Impact on molecular electronics research

A.Vollmer¹, R. Ovsyannikov¹, M. Gorgoi¹, S. Krause¹, M. Oehzelt¹, A. Föhlisch¹, A. Lindblad², N. Martensson², S. Svensson², P. Karlsson³, M. Lundquist³, T. Schmeiler⁴, J. Pflaum⁴, and N. Koch^{1,5}

1 Helmholtz Zentrum Berlin für Materialien und Energie GmbH, Institut für Methoden und Instrumentierung der Forschung mit Synchrotronstrahlung, 12489 Berlin, Germany

2 Institute for Physics and Astronomy, Uppsala University, Sweden

3 VG Scienta AB, P.O. Box15120, SE-750 15 Uppsala, Sweden

4 Lehrstuhl für Experimentelle Physik VI, Universität Würzburg and ZAE Bayern, 97074 Würzburg, Germany

5 Institut für Physik, Humboldt-Universität zu Berlin, 12489 Berlin, Germany

E-mail: antje.vollmer@helmholtz-berlin.de

We report on a novel type of photoemission instrument, the Angle Resolved Time Of Flight electron energy analyzer (ARTOF 10k), a time-of-flight electron spectrometer which combines position-sensitive detection with an advanced focusing electron lens system. The instrument facilitates the simultaneous recording of kinetic energy and angular pattern of photoelectrons in a cone of up to 30° opening angle with very high energy resolution at unchanged geometrical conditions throughout the whole experiment. Compared to state of the art instruments the resolution is improved to the theoretical limit of about 100 μeV and the transmission is increased by a factor of more than 250 [1,2]. This allows for very mild conditions during the experiment turning the ARTOF 10k into the predestined instrument to investigate specimens that strongly suffer from radiation damage during photoemission experiments under "standard" conditions, such as organic single crystals, as extremely low fluxes can be used while not compromising spectra accumulation times. Even though organic single crystals are of increasing fundamental and applied scientific interest, knowledge of their electronic properties is still mainly based on theoretical calculations due to major experimental challenges in measuring photoemission. Here we present the band structures of rubrene and tetracene single crystals obtained with unprecedented quality using the ARTOF instrument within only a few hours of measurement time.

References

- [1] G. Öhrwall, *et al.*, J. Electron Spectrosc. **183** (2011) 125.
- [2] P.D.C: King *et al.*, PRL **107**, (2011) 096802.

Interaction at hetero-epitaxial organic interfaces: Phthalocyanine and PTCDA molecules on noble metal surfaces

Christian Kumpf ^{1,2}

¹ *Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany.*

² *Jülich-Aachen Research Alliance – Fundamentals of Future Information Technologies (JARA-FIT)*

E-mail: c.kumpf@fz-juelich.de

The properties of functional materials and electronic devices are dominated by their surfaces and interfaces. This is particularly true for organic thin films and adsorbate systems. While recently interfaces between organic layers and metals were investigated intensively, only very few studies focus on the interface between different organic materials.

Model systems in this context are copper-II-phthalocyanine (CuPc) and perylen-tetra-carboxylicacid dianhydride (PTCDA) on Ag, Au and Cu(111) surfaces, which we have studied intensively in a multiple technique approach. The hetero-epitaxial system CuPc/PTCDA is of particular interest since it combines two molecules exhibiting very different structure formation mechanisms: While PTCDA forms well-ordered island on the Ag(111) surface, caused by an attractive intermolecular interaction, CuPc molecules repel each other after adsorption and form dilute phases [1-4].

In this talk we are going to give an overview of our experiments on these model systems using high resolution low energy electron diffraction (SPA-LEED), X-ray and UV photo-electron spectroscopy (XPS, UPS), x-ray standing waves (XSW) and scanning tunneling microscopy (STM).

References

- [1] C. Stadler, S. Hansen, I. Kröger, E. Umbach, C. Kumpf, *Nature Physics* **5**, 153 (2009).
- [2] I. Kröger, B. Stadtmüller, C. Stadler, J. Ziroff, M. Kochler, A. Stahl, F. Pollinger, T.-L. Lee, J. Zegenhagen, F. Reinert, C. Kumpf, *New J. Phys.* **12**, 083038 (2010).
- [3] B. Stadtmüller, I. Kröger, F. Reinert, C. Kumpf, *Phys. Rev. B* **83**, 085416 (2011).
- [4] I. Kröger, B. Stadtmüller, C. Kleimann, P. Rajput, C. Kumpf, *Phys. Rev. B* **83**, 195414 (2011).

4-2A

Theoretical study of dipole layer formation at organic/metal interfaces

Yoshitada Morikawa¹, Kenji Toyoda², Ikutaro Hamada³, and Susumu Yanagisawa⁴

¹*Department of Precision Science and Technology, Osaka University*

²*Advanced Technology Research Laboratories, Panasonic Corporation*

³*WPI-Advanced Institute for Materials Research, Tohoku University*

⁴*Department of Physics and Earth Sciences, University of the Ryukyus*

E-mail: morikawa@prec.eng.osaka-u.ac.jp

In order to clarify factors determining the interface dipole, we have studied the electronic structures of benzene, pentacene, and perfluoropentacene adsorbed on Cu, Ag, and Au surfaces by using first-principles density-functional theoretical calculations [1-5]. In the structural optimization, the semi-empirical van der Waals (vdW) approach [6] is employed to include long-range vdW interactions, and is shown to reproduce pentacene-metal distances quite accurately. The pentacene-metal distances for Cu, Ag, and Au are evaluated to be 0.24, 0.29, and 0.32 nm, respectively, and work function changes calculated by using the theoretically optimized adsorption geometries are in good agreement with the experimental values, indicating the validity of the present approach in the prediction of the interface dipole at metal/organic interfaces. We examined systematically how the geometric factors, especially the pentacene-substrate distance (Z_C), and the electronic properties of the metal substrates contribute to the interface dipole. We found that at $Z_C > 0.35$ nm, the work function changes ($\Delta\phi$'s) do not depend on the substrate work function (ϕ_m), indicating that the interface level alignment is nearly in the Schottky limit, whereas at $Z_C < 0.25$ nm, $\Delta\phi$'s vary nearly linearly with ϕ_m and the interface level alignment is in the Bardeen limit. Our results indicate the importance of both the geometric and the electronic factors in predicting the interface dipoles.

References

- [1] K. Toyoda, Y. Nakano, I. Hamada, K. Lee, S. Yanagisawa, and Y. Morikawa, *J. Electron Spectrosc. Relat. Phenom.* **174**, 78 (2009).
- [2] K. Toyoda, Y. Nakano, I. Hamada, K.H. Lee, S. Yanagisawa, and Y. Morikawa, *Surf. Sci.*, **603**, 2912-2922 (2009).
- [3] K. Toyoda, I. Hamada, S. Yanagisawa, and Y. Morikawa, *Appl. Phys. Express*, **3**, 025701 (2010).
- [4] K. Toyoda, Y. Nakano, I. Hamada, K. Lee, S. Yanagisawa, and Y. Morikawa, *J. Chem. Phys.*, **132**, 134703 (2010).
- [5] K. Toyoda, I. Hamada, S. Yanagisawa, and Y. Morikawa, *Organic Electronics*, **12**, 295-299 (2011).
- [6] K. Toyoda, I. Hamada, K.-H. Lee, S. Yanagisawa, and Y. Morikawa, *J. Phys. Chem. C*, **115**, 5767-5772 (2011).
- [7] K. Toyoda, I. Hamada, S. Yanagisawa, and Y. Morikawa, *J. Nanoscience and Nanotech.*, **11**, 2836 (2011).
- [8] S. Grimme, *J. Comput. Chem.* **27**, 1787 (2006).

Giant surface potential due to spontaneous noncentrosymmetric molecular orientation in vacuum-deposited thin film of Alq₃ derivatives

Takashi ISOSHIMA¹, Eisuke ITO¹, Youichi OKABAYASHI¹, Whee Won CHIN²,
Jin Wook HAN², Masahiko HARA¹

¹*Flucto-Order Functions Research Team, RIKEN-HYU Collaboration Research Center, RIKEN
Advanced Science Institute, Japan*

²*Department of Chemistry, Hanyang University, Korea*

E-mail: isoshima@riken.jp

Tris(8-hydroxyquinolinato) aluminum (III) (Alq₃) and similar ML₃-type compounds (M: metal, L: organic ligand) are organic semiconductors popularly used in various organic devices. These materials are often employed as vacuum-deposited thin films. Molecular orientation in the film is important since it affects optical and electric properties. Alq₃ and ML₃-type materials are known to present spontaneous huge surface potential when vacuum-deposited in dark [1]. The surface potential is linearly proportional to the film thickness as large as 50 V/μm, hence called giant surface potential (gSP). gSP originates from polar (noncentrosymmetric) molecular orientation in the amorphous thin films. It is also known that gSP reduces by irradiation of visible light. In this presentation, we describe our investigation on the spontaneous polar molecular orientation and gSP phenomenon in Alq₃ and related materials.

Polar molecular orientation can be investigated through 2nd-order nonlinear optical measurement. We employed the 1st-order electroabsorption (EA) spectroscopy. The order parameter of molecular orientation was evaluated to be *ca.* 0.01 even after photoinduced reduction of gSP, indicating that the reduction originates from electrostatic screening by photocarrier. We investigated dependence of gSP and molecular orientation on deposition conditions and on substrate materials, but the dependence was small. This suggests that interfacial interaction is not a critical factor to determine the molecular orientation. On the other hand, we found that chemical structure of the molecule significantly affects gSP and polar molecular orientation. Peripherally substituted Al(5-Clq)₃ presented about twice as high gSP, and Al(7-Prq)₃ (Pr=propyl) presented *negative* gSP. These results suggest controllability of magnitude and polarity of gSP and molecular orientation by chemical modification. These facts are important in terms of elucidation for spontaneous molecular orientation and also interesting in applications, enabling us to control interfacial electronic properties and nonlinear optical properties.

References

[1] E. Ito, Y. Washizu, N. Hayashi, H. Ishii, N. Matsuie, K. Tsuboi, Y. Ouchi, Y. Harima, K. Yamashita, and K. Seki, *J. Appl. Phys.*, **92**, 7306 (2002).

5-1A

Organic and hybrid organic heterojunctions in organic electronics and spintronics applications

Slawomir Braun,¹ L.M. Andersson,¹ P. Sehati,¹ Y.Q. Zhan,^{1,2} M.P. de Jong,³ Mats Fahlman¹

¹*Department of Physics, Chemistry and Biology, Linköping University, Sweden.*

²*Microelectronics Department, IT School, Fudan University Shanghai, China*

³*MESA+ Institute for Nanotechnology, University of Twente, Enschede, the Netherlands*

E-mail: mafah@ifm.liu.se

Organic electronic and spintronic devices such as solar cells and spin valves are multi-layered devices where their ultimate performance is to a large extent dominated by the electronic processes at interfaces. The relative position of energy levels across a stack of thin organic layers is important for charge/spin injection and exciton separation, and hence for device engineering and optimization. Here we will present some recent results on P3HT and PCBM where we explore the effects of inter- and intra-molecular order at the interface on the $E_{ICT+,-}$ and how these parameters affect exciton dissociation and charge transport [1]. In the latter case P3HT, both in a well ordered state and with temperature induced disorder, is characterized and analyzed in terms of the ICT model, the Gaussian disorder model and a simple polaronic approach consistent with Marcus theory. In a separate set of experiments we explore so-called spinterfaces, where the energy level alignment and spin-polarization of the molecular orbitals of π -conjugated molecules are studied for the Alq₃/Fe and C₆₀/Fe systems. We demonstrate hybridization and exchange coupling between a π -conjugated orbital in Alq₃ molecules adsorbed on the Fe surface. The hybridization results in an Ohmic-like contact and efficient charge injection. Furthermore, the exchange coupling induces spin-polarization of a π -conjugated orbital in Alq₃, which enable the efficient spin injection [2]. For the C₆₀/Fe system, hybridization between the frontier orbitals of C₆₀ and continuum states of Fe leads to a significant magnetic polarization of C₆₀ π^* -derived orbitals. The magnitude and also the sign of this polarization were found to depend markedly on the excitation energy [3].

References

- [1] Harri Aarnio, et al, Adv. Energy Mater, **1**, 792 (2011).
- [2] Yiqiang Zhan, et al, Adv. Mater., **22**, 1626 (2010).
- [3] T.L.A. Tran, et al, Appl. Phys. Lett., **98**, 222505 (2011).

Electronic structure of a cobalt-phthalocyanine adsorbed quasi-one dimensional Ag surface

Yusuke Tanaka¹, Puneet Mishra², Ryusei Tateishi³, Nguyen Thanh Cuong^{4,5}, Hideo Orita⁵, Minoru Otani^{4,5}, Tomonobu Nakayama², Takashi Uchihashi², Kazuyuki Sakamoto³

¹*Department of Chemistry, Nagoya University, Nagoya 464-8602, Japan*

²*National Institute for Materials Science, Namiki 1-1, Tsukuba 305-0044, Japan*

³*Department of Nanomaterials Science, Chiba University, Chiba 263-8522, Japan*

⁴*National Institute of Advanced Industrial Science and Technology, Umezono1-1-1, Tsukuba 305-8568, Japan*

⁵*JST-CREST, 5 Sanbancho, Chiyoda-ku, Tokyo 102-0075, Japan*

E-mail: kazuyuki_sakamoto@faculty.chiba-u.jp

Fabrication of organic molecule nanostructures with tailored morphology as well as electronic property is an important aspect of current nanotechnology research [1]. In this paper, we report the adsorption structure and the electronic states of cobalt-phthalocyanine (CoPc) wires grown on a striped Ag substrate [2]. By using low-temperature scanning tunneling microscopy, we observed the formation of 1D CoPc chains along the striped structure of the Ag substrate. Regarding the electronic states, quantum confinements of 1D surface states electron by organic molecules were observed. The change in intermolecular distance leads to a change in the quantum confinement, indicating that the confinement depends on the size of the potential box. The observation of site-specific standing waves formed by CoPc molecules revealed that the Pc ring of CoPc molecule scatters the surface states electron of the striped Ag substrate, and works as a potential wall even though the π orbitals of a Pc ring in CoPc molecule is supposed to weakly adsorb onto the Ag surface. We will also present detailed analysis performed using the phase accumulation model, and demonstrate the energy dependence of the phase shift at CoPc molecules and that of the standing waves penetration into a CoPc molecule.

References

[1] J.V. Barth *et al.*, Nature **437** (2005) 671; C. Tegenkamp, J. Phys.: Condens. Matter **21**, 013002 (2009).

[2] T. Uchihashi *et al.*, PRL **96**, 136104 (2006).

5-3L

Theoretical proposal for indirect measurement of weakly-coupled adsorbates on quasi-1D metallic substrate by STS

Masayuki Yamamoto

Department of Nanomaterials Science, Chiba University, Chiba 263-8522, Japan
E-mail: myamamoto@graduate.chiba-u.jp

Direct measurement of molecular adsorbates by UPS (as well as STS) accompanies an ionization of adsorbates, which can affect the position and shape of observed spectra. In this talk, we propose a possible way to access the energy levels of weakly-coupled adsorbate without ionization, that is the STS measurement of the interference pattern between an incoming wave and a scattered one by adsorbates on quasi-one dimensional metallic substrate. It is known that, in a nanowire with a side-coupled quantum dot, the Fano resonance occurs when the energy of conduction electrons in nanowire varies across the discrete energy levels of quantum dot [1]. This resonance induces the rapid π -phase shift of a scattered wave as well as a transmitted one. Thus the interference pattern between incoming and scattered waves should also show the shift at the energy levels of a coupled state. We have numerically confirmed such a shift of interference pattern at least in a simple one-dimensional discrete lattice model. The experimental realization may be possible by using STS and quasi-one dimensional metallic substrate [2].

References

- [1] K. Kobayashi *et al.*, PRB **70**, 035319 (2004).
- [2] T. Uchihashi *et al.*, PRL **96**, 136104 (2006).

Electronic excitation of rubrene/HOPG mediated by image potential state

T. Ueba¹, J. Park², R. Terawaki¹, T. Yamada¹, H. S. Kato¹, and T. Munakata¹

¹Graduate School of Science, Osaka University, Toyonaka 560-0043, Japan,

²Department of Chemistry, Seoul National University, Seoul 151-747, Korea,

E-mail: munakata@chem.sci.osaka-u.ac.jp

Electronic excitation of adsorbed molecules typically occurs by intra-molecular excitation and/or by electron transfer from the substrate. Here we report a new path causing the electronic excitation of molecules: image potential state (IPS) mediated excitation. IPS is the Rydberg-like unoccupied state supported in between the Coulombic image potential and the band gap of the substrate. The first member ($n=1$) of the state on HOPG is located at 0.85 eV below the vacuum level and behaves as 2D free electron of $m^*/m_e=1.1$ [1]. The 2D electron located outside the surface is repelled by PbPc molecules and shows lateral confinement at sub-ML coverages [2]. The interaction of IPS with rubrene molecule is largely different from that with PbPc. We have performed two-photon photoemission (2PPE) spectroscopy for rubrene/HOPG as shown in Fig.1. The peaks labeled by Ln , IPS1, and IPS2 are assigned to a molecule-derived unoccupied state, IPS on bare HOPG, and IPS on the molecular film, respectively. The peak labeled H, shifting at $h\nu < 4.38$ eV, arises from the direct 2PPE from the HOMO at -1.08 eV initial energy. At $h\nu > 4.38$ eV, the H peak disappears and the Ln peak appears. The intensity switching at the resonance is the general trend in 2PPE [3]. It is interesting that the intensity of the Ln peak becomes maximum at $h\nu = 4.45$ eV, higher than the resonance. The enhancement of Ln peak becomes less significant as the IPS1 peak disappears at coverage higher than 1 ML as shown in Fig.2. The enhancement is suppressed with s-polarization. These suggest that the enhancement of the Ln peak is mediated by the substrate IPS1. IPS1 orbital interacts with the Ln orbital at the edges of molecular domains, and causes the strong resonance enhancement.

References

- [1] J. Phys. Chem. C, in press.
- [2] Surf. Sci., 605, 982-986 (2011).
- [3] Phys. Rev. B 81, 115426(1-8) (2010).

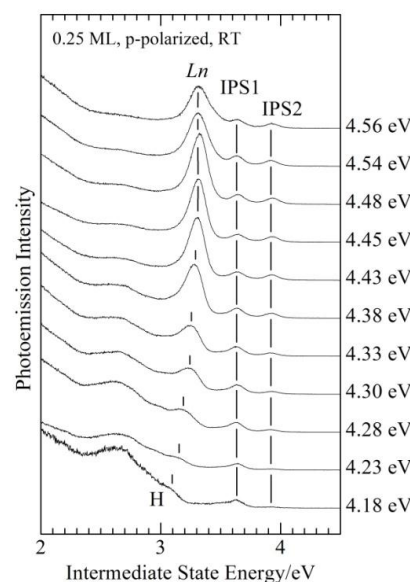


Fig.1 $h\nu$ dependent 2PPE spectra

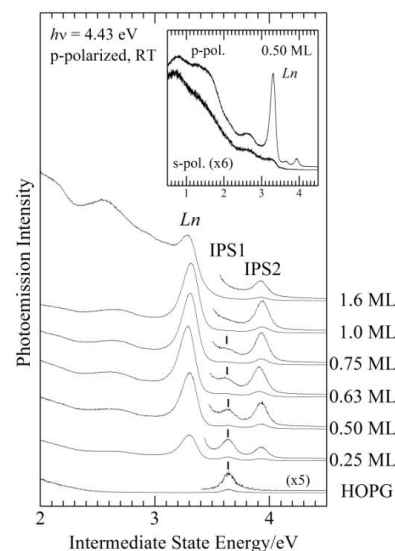


Fig.2 Coverage dependence

6-2A

Development of the HELIOS laboratory for time-resolved VUV/soft X-ray pump-probe studies at Uppsala University, Sweden

Johan Söderström¹, Stefan Plogmaker¹, Joachim Rausch¹, Jan-Erik Rubensson¹, Hans Siegbahn¹

¹*Department of Physics and Astronomy, Uppsala University, Box 516, 751 20 Uppsala, Sweden*
E-mail: Johan.Soderstrom@physics.uu.se

During the last decades synchrotron radiation has been a very powerful tool to investigate properties of matter, ranging from gas-phase, solid phase and even encompassing liquid phases. Synchrotron based experiments have drastically improved much because of the improved instrumentation used, such as higher quality of optics and detection schemes used. The increased photon flux has given researchers the possibility to access more dilute samples, and the increased experimental resolution shows even finer details on an almost yearly basis.

One branch where synchrotron based research has not been a strong competitor is in the field of time resolved pump-probe experiments, during the latest years this has been changing, by use of so-called slicing-techniques at synchrotrons, Free Electron Lasers (FELs) and Higher Harmonic Generation (HHG) techniques. I will present the HELIOS (High Energy Laser Induced Overtone Source) laboratory currently being built in Uppsala, Sweden based on the HHG technique. At HELIOS we aim to do provide pump-photons with a wavelength between 285 and 20 000 nm and probe photons with energies between 10 and 100 eV.

I will present the overall goals, the design – which strongly focuses on retaining a high temporal resolution (<35 fs) for the VUV photons and the first proof-of-principle experiments performed in the fall of 2011.

The photoconductivity of pentacene thin films as a function of thickness

Richard Murdey and Naoki Sato

Institute for Chemical Research, Kyoto University, Uji, Kyoto, Japan 611-0011

E-mail: rmurdey@e.kuicr.kyoto-u.ac.jp

Photocurrents in pentacene thin films were measured *in situ* as a function of film thickness from 5 nm to 100 nm. The films were vacuum-deposited on single-crystal sapphire [0001] substrates patterned with Au electrodes. Photoaction spectra were obtained at 10^5 V m⁻¹ over excitation wavelengths 1180 nm – 400 nm using a Bunkokeiki SM-25 monolight and Keithley 6487 picoammeter/sourcemeater. Film growth and measurements were performed at room temperature under a typical operating vacuum of 10^{-6} Pa.

For the pentacene films in the thickness range of 5–30 nm the dark conductance increases linearly with film thickness and the conductivity can be estimated at 6.2×10^{-8} S m⁻¹; dark conductance was confirmed to be Ohmic for the field strength used. The thermal activation energy of conductivity in the temperature range of 30 – 75 °C was found to be 0.75 eV. The onset of photoconductance is 1.7 eV, the same as the optical gap, and the photoconductance signal for the films corresponds closely to the $S_1 \rightarrow S_0$ singlet exciton transition in the optical absorption spectra. A peak at about 2.7 eV which is not observed in the optical absorption spectra gradually increases in intensity with increasing film thickness. A similar peak was previously observed in pentacene single crystals [2]. It was identified by these authors as the intrinsic band-to-band transition across the HOMO-LUMO-derived (transport) energy gap.

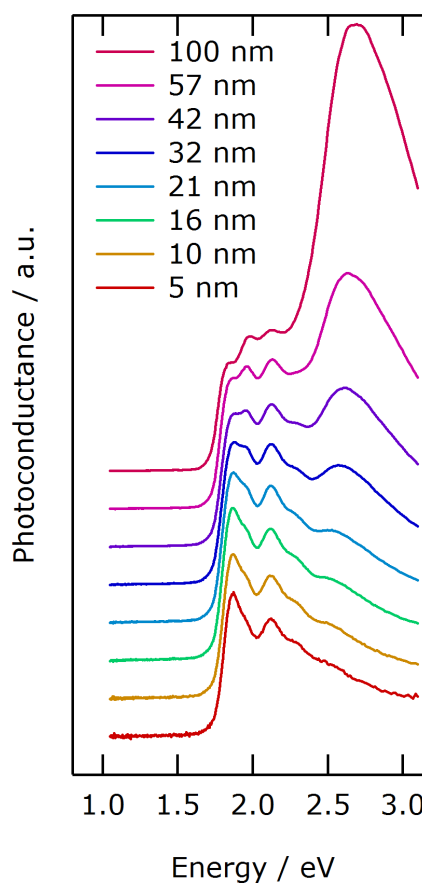


Fig. 1. Photoconductance spectra for various pentacene film thicknesses. Offset for clarity.

References

- [1] C. Jundt et al., *Chem. Phys. Lett.*, **241**, 84 (1995); J. Burgos, *Phys. Stat. Sol. B.*, **83**, 249 (1977).
- [2] D.V. Lang et al., *Phys. Rev. Lett.*, **93**, 086802 (2004).

7-1A

Spin-polarized current through graphene nanoflake

Tomoya Ono

Graduate School of Engineering, Osaka University
E-mail: ono@prec.eng.osaka-u.ac.jp

Graphene, as a two-dimensional monolayer honeycomb structure of carbon, is known to exhibit a rich variety of electronic structures and is expected to be one of the most promising new materials for future nanoelectronics. The discovery of zigzag graphene nanoribbons, in which an opposite spin orientation crosses the ribbon between ferromagnetically ordered edge states on each edge, through theoretical calculations has attracted a great deal of interest in spintronics applications based on graphene based materials. Okada and Oshiyama[1] studied the spin polarizations of two dimensional structures composed of boron, nitrogen, and carbon, in which triangular graphene flakes is surrounded by boron nitride (BN) sheets (referred to as BNC structures after this), through first-principles calculations and found that flat-band states can be observed around the Fermi level and the BNC structures are ferromagnetically polarized.

In this study, I have examined the electronic structures and transport properties of graphene flakes surrounded by BN sheet as shown in Fig. 1 by first-principles electronic structure and transport calculations.[2,3,4] I found that the magnetic moment of the graphene flakes increases as the flakes become small and as they become isolated. When the BNC structure is connected to graphene electrodes, the spin polarization of the charge density distribution accumulates at the edges of the flakes and no spin polarizations are observed in the graphene electrodes. First-principles transport calculation revealed that electron transport through the BNC structure is fully polarized in a wide energy range around the Fermi level. These results should stimulate interest in spintronics devices using carbon-based materials and a bottom-up technology.

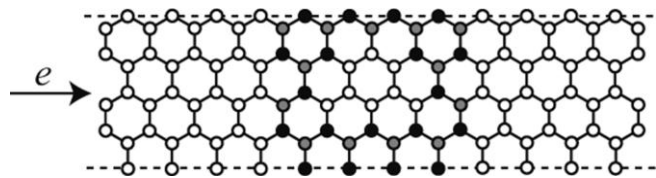


Fig. 1. Computational model for spin-polarized current through a triangular flake.

References

- [1] S. Okada, A. Oshiyama, *Phys. Rev. Lett.* **87**, 146803 (2001).
- [2] Y. Fujimoto, K. Hirose, *Phys. Rev. B* **67**, 195315 (2003).
- [3] T. Ono, K. Hirose, *Phys. Rev. B* **70**, 033403 (2004).
- [4] K. Hirose, T. Ono, Y. Fujimoto, S. Tsukamoto, *First-Principles Calculations in Real-Space Formalism-Electronic Configurations and Transport Properties of Nanostructures-*; Imperial College Press: London, UK, 2005.

Interfacial electronic properties between organic semiconductor and graphene films

Xianjie Liu¹, Alexander Grueneis²

¹*Department of Physics, Chemistry and Biology, Linköping University, Sweden.*

²*Faculty of Physics, Univeristy of Vienna, 1090, Wien, Austria*

E-mail: xjliu@ifm.liu.se

Owing to their unique mechanical and electronic properties, graphene have gained tremendous interests related to their perspective in applications. The extremely high mobility and light transparency of graphene make it as one of promising candidates of flexible electrode for organic electronics. Here we present our recent studies of interfacial properties between organic semiconductor pentacene and monolayer graphene film. Since all synthetic graphene films are supported by different substrates like Ni/Cu, SiC, they are far from real free-standing. The influence of the substrate upon electronic properties between organic and graphene should be addressed when molecules are adsorbed. Graphene films from different growth sources and substrates, intercalation, and modification were taken in the study. We focus on the molecular orientation of pentacene upon dirty and clean graphene films with angle-dependent x-ray absorption spectroscopy, then demonstrate how to tune the molecular orientation by inserting monolayer F₁₆CuPc between graphene and pentacene. Correspondingly, the related energy level alignment between organic and graphene will be discussed.

7-3A

Structural and electronic properties of epitaxial silicene

Yukiko Yamada-Takamura, Antoine Fleurence, Taisuke Ozaki, Ying Wang, Fabio Bussolotti, and Rainer Friedlein

*School of Materials Science and Research Center for Integrated Science,
Japan Advanced Institute of Science and Technology (JAIST),
1-1 Asahidai, Nomi, Ishikawa 923-1292, Japan,
E-mail: yukikoyt@jaist.ac.jp*

The experimental realization of extended, two-dimensional sheets of silicene, the silicon counterpart of graphene, has been elusive so far. Here, we demonstrate that such a two-dimensional, epitaxial honeycomb Si layer forms through surface segregation on a metallic zirconium diboride (ZrB_2) film grown itself epitaxially on Si(111) [1]. The honeycomb Si layer uniformly covers the $\text{ZrB}_2(0001)$ surface forming a (2×2) reconstruction. Surface-sensitive core-level photoelectron spectroscopy and photoelectron diffraction performed using a photon energy of 130 eV identifies Si atoms in different chemical states that are either in contact with Zr atoms or not, confirming details of the slightly-buckled honeycomb structure obtained through scanning tunneling microscopy. Angle-resolved ultraviolet photoelectron spectra reflect surface electronic states related to the π band structure of slightly-buckled, free standing silicene together with those of the uppermost Zr layer.

Such epitaxial silicene allows the integration of silicon-based and organic electronics for high mobility and high frequency applications. The surface chemical properties of silicene allow the direct growth of ordered organic films, which is impossible on bulk silicon, as our initial experiments with anthracene and pentacene show.

References

[1] Y. Yamada-Takamura, F. Bussolotti, A. Fleurence, S. Bera, R. Friedlein, Appl. Phys. Lett. **97**, 073109 (2010).

8-1S

Charge transport in organic semiconductors: A theoretical perspective

Veaceslav Coropceanu, Yuan Li, and Jean-Luc Brédas

Center for Organic Photonics and Electronics and School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA 30332-0400, USA

E-mail: coropceanu@gatech.edu

In this contribution, we discuss state-of-the-art quantum-chemical approaches used to derive the microscopic parameters and model the charge-transport properties in organic molecular semiconductors. In these systems, there exist two major electron-phonon coupling mechanisms: The first is referred to as local coupling and arises from the modulation of the site energy by vibrations (Holstein-type coupling); the second mechanism, the nonlocal coupling, comes from the modulation of the transfer integrals by vibrations (Peierls-type coupling). The impact on the charge-transport characteristics of the interplay between these two types of electron-phonon coupling is investigated in the framework of band, disorder, and semi-classical models. Our results show that, for an adequate description of charge transport in organic semiconductors, both electron-phonon mechanisms should be taken into account. We compare our findings to recent experimental data.

8-2A

Insight into the HOMO hole in π -conjugated molecules as dielectric medium

Satoshi Kera¹ and Nobuo Ueno¹

¹*Graduate School of Advanced Integration Science, Chiba University, Chiba, Japan,*
E-mail: kera@faculty.chiba-u.jp

Binding energy, vibration coupling, density-of-states and lifetime related phenomena of the highest occupied molecular orbital (HOMO) state in a thin film of organic semiconductor play a crucial role in the hole transport through the film and the charge transfer from an electrode to the ionized molecule. The line shape of the HOMO band in highly resolved UPS spectra in principle involves all of these contributions, and thus offers a variety of key information that is necessary to unravel fundamental mechanism in carrier-transport properties in organic devices. Here, we present our longstanding high-resolution but *conventional* UPS studies on the HOMO hole in monolayers of phthalocyanines and pentacene [1-4]. The results may give a chance to address the origin of the HOMO-band shape for molecular solids that is related to following phenomena: (i) hole-vibration coupling which was experimentally observed for organic molecular monolayers on conductive substrates to give an asymmetric HOMO shape. (ii) dynamic properties of polarization (polaron related phenomena) and effects of the photohole lifetime that give a higher-kinetic energy tail in the HOMO shape.

References

- [1] S. Kera et al, *Chem. Phys. Lett.* 364, 93 (2002).
- [2] H. Yamane et al., *Phys. Rev. B* 72, 153412 (2005).
- [3] N. Ueno and S. Kera, *Prog. Surf. Sci.* **83**, 490 (2008).
- [4] S. Kera, H. Yamane and N. Ueno, *Prog. Surf. Sci.* **84**, 135 (2009).

Charge reorganization energy and small polaron binding energy of rubrene thin films by UPS

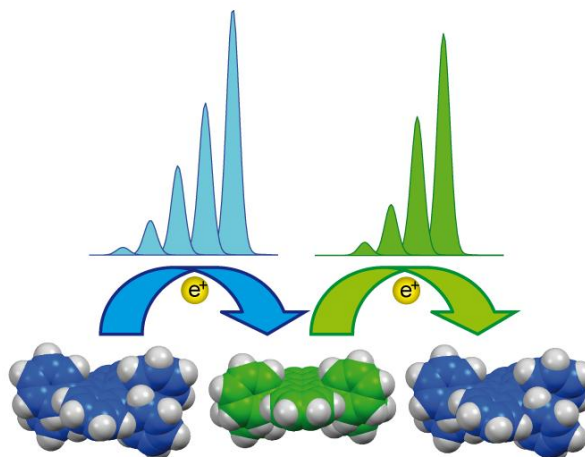
Steffen Duhm¹, Qian Xin¹, Shunsuke Hosoumi¹, Hirohiko Fukagawa^{1,2}, Kazushi Sato¹, Nobuo Ueno¹ and Satoshi Kera¹

¹Graduate School of Advanced Integration Science, Chiba University, Chiba, Japan,

²Present address: NHK Science and Technical Research Laboratories, Tokyo, Japan

E-mail: duhm@restaff.chiba-u.jp

One major drawback of *Organic Electronics* is the low charge carrier mobility in most organic thin films and organic single crystals. However, rubrene single crystals exhibits outstanding hole mobilities. Recently, we could demonstrate band like transport and a surprisingly low effective mass of the HOMO hole ($m^* = 0.65 m_0$) in rubrene single crystals using angle resolved ultraviolet photoelectron spectroscopy (ARUPS) [1]. In order to study the peculiar charge carrier phonon coupling of solid rubrene and thus the charge reorganization energy λ , which is a key parameter for the hopping mobility in organic thin films and crystals [2], we measured ARUPS of vacuum-sublimed rubrene thin films on graphite (HOPG). The charge reorganization energies of rubrene monolayers on HOPG are 155 meV for a conformation with a twisted backbone and 157 meV for a conformation with a planar backbone, which coexist in the monolayer. Both values are smaller than λ in the gas phase, which is in contrast to other prototypical organic semiconductors like pentacene and might be one key to explain the transport properties of rubrene thin films and single crystals. Moreover, the present results also offer the binding energies of the small polaron for the two conformations with 78 meV and 79 meV, respectively.



References

- [1] S. Machida, Y. Nakayama, S. Duhm, Q. Xin, A. Funakoshi, N. Ogawa, S. Kera, N. Ueno and H. Ishii, *Phys. Rev. Lett.* **104**, 156401 (2010).
- [2] S. Kera, H. Yamane and N. Ueno, *Prog. Surf. Sci.* **84**, 135 (2009).

9-1A

Multi-scale transport calculations for nanomaterial systems

Kenji Hirose¹, Hiroyuki Ishii², and Nobuhiko Kobayashi²

¹*Green Innovation Research Laboratories, NEC Corporation.*

²*Institute of Applied Physics, University of Tsukuba*

E-mail: hirose@ak.jp.nec.com

We present our recent activities of electron transport calculations for nanomaterial systems. Using different computational methods such as recursion-transfer-matrix (RTM) method, non-equilibrium Green's function (NEGF) method, and time-dependent wave-packet diffusion (TD-WPD) method, which constitute the multi-scale transport calculations, we present the contact effects of molecules to metallic electrodes on electron transport, transition from diffusive to ballistic transport by the electron-phonon scatterings and phase coherence problem of carbon nanotubes, and others.

Intermolecular interaction in crystalline films of phthalocyanines probed by high-resolution photoelectron spectroscopy

Hiroyuki Yamane, Nobuhiro Kosugi

Institute for Molecular Science, Myodaiji-cho, Okazaki 444-8585, Japan
E-mail: yamane@ims.ac.jp

Recently, we have developed a high-resolution angle-resolved UV/SX photoelectron spectroscopy (ARPES) system at a high-brilliant in-vacuum soft-X-ray undulator beamline UVSOR BL6U, which covers the photon energy ($h\nu$) of 40–600 eV with the resolving power ($E/\Delta E$) of 10000 at $h\nu = 400$ eV. The ARPES system consists of an analysis chamber, sample preparation chamber, and load-lock chamber. In the analysis chamber, we have installed a (i) high-resolution electron analyzer (MBS-A1), (ii) liquid-He flow cryostat with a compact 5-axes manipulation (x, y, z, polar, and $\pm 90^\circ$ -azimuth) system, and (iii) low-energy electron diffraction optics with a micro-channel plate.

In this contribution, we discuss the intermolecular interaction in metal phthalocyanines (MPc) based on our ARPES observation of the intermolecular valence band dispersion in crystalline films of MPc (e.g., ZnPc, F_{16} ZnPc, and MnPc). In the case of ZnPc (Fig. 1), we found that the transfer integral for the highest occupied molecular orbital (HOMO) band of the π character is about 25 meV at 15 K. The present observation clearly indicates that the band-like transport can be realized even in the evaporated MPc films by the control of the geometric film structure. Moreover, the present result can be a benchmark for the systematic study on the intermolecular interaction, e.g., intermolecular valence band dispersion as a function of the central metal atom in the molecule, which enables to discuss the intermolecular interaction in terms of the intermolecular distance and the molecular orbital symmetry.

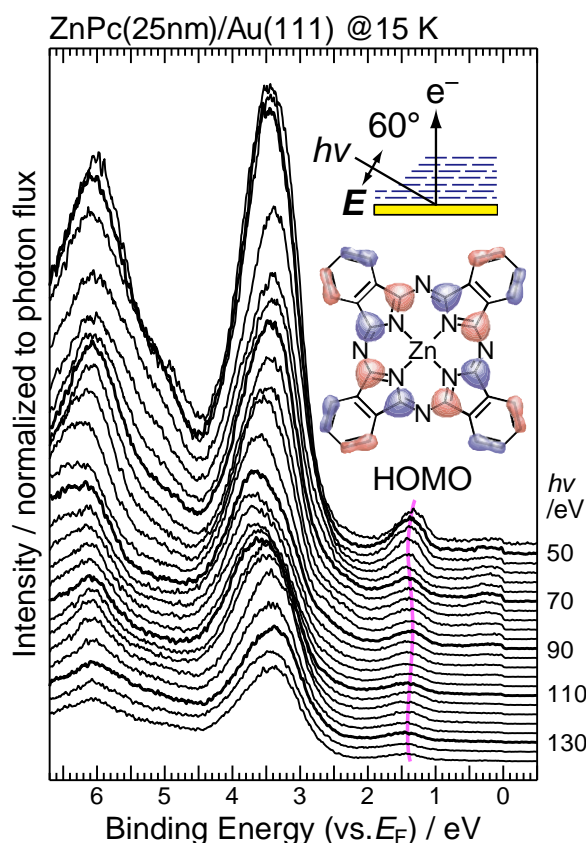


Fig. 1. The photon energy ($h\nu$) dependence of the normal-emission ARPES spectra ($h\nu$ step = 4 eV) of the ZnPc crystalline film prepared on the Au(111) surface.

9-3L

Pentacene thin film on SiO₂ substrate: Electronic properties vs. growth conditions

F. Bussolotti¹, S. Kera¹, N. Ueno¹

¹Graduate School of Advanced Integration Science, Chiba University, Chiba 263-8522
E-mail: fabio@restaff.chiba-u.jp

Over the last three decades, organic molecular semiconductors have attracted increasing scientific attention due to their interesting chemical, optical, and electrical properties[1]. The possibility of processing large areas at low cost, light weight, mechanical flexibility, makes organic molecular semiconductors suitable materials for the development of a wide range of solid-state electronic and optoelectronic devices [2]. Considerable research efforts have therefore been devoted to understand the nature of charge transport mechanisms in organic molecular crystals and thin films of varying degrees of molecular order and molecular orientation as well to the electronic properties at the organic/substrate interface [3,4].

In this context, the electronic properties of Pentacene (C₂₂H₁₄) thin film on Silicon oxide substrate (a prototype system for a wide range of organic based electronic devices) have been investigated by using High Resolution-Ultra Low background Photoelectron Spectroscopy. In particular, by tuning the substrate temperature during the growing process, organic thin film with different degree of structural order have been obtained. The impact of the structural disordering on the energy level alignment at the organic substrate interface and on the density of state distribution have been carefully discussed.

Analogous study on the effect of the N₂ exposure on the electronic properties of Pn organic thin film will be presented and discussed.

References

- [1] G. Horowitz, *J. Mater. Research* **19**, (1946).
- [2] M. Halik, H. Klauk, U. Zschieschang, T. Kriem, G. Schmid, W.Radlik, and K. Wussow, *Appl. Phys. Lett.* **81**, 289 (2002).
- [3] T. Hosokai, H. Machida,A. Gerlach, S. Kera, F. Schreiber, and N. Ueno *Phys. Rev. B* **83**, 195310 (2011).
- [4] T. Sueyoishi, H. Kakuta, M.Ono, K. Sakamoto, S. Kera, N. Ueno, *Appl. Phys. Lett.* **96**, 093303 (2010).

Extended electronic states in self-assembled genetic matter

Rainer Friedlein, Ying Wang, Antoine Fleurence, Yukiko Yamada-Takamura

*School of Materials Science, Japan Advanced Institute of Science and Technology, 1-1 Asahidai,
Nomi, Ishikawa 923-1292, Japan,
E-mail: friedl@jaist.ac.jp*

Templated supramolecular self-assembly based largely on hydrogen bonding between relatively small heterocyclic molecules forms the basis of life and may be a powerful tool to achieve new organic electronic materials with excellent transport properties [1].

Here, we review our recent progress in growing highly-ordered multilayer films of the nucleic acids guanine, adenine, thymine and cytosine as well as of guanine-cytosine Watson-Crick pairs in a layer-by-layer fashion on the surface of highly-oriented pyrolytic graphite. As revealed by synchrotron-based photon-energy dependent photoelectron spectroscopy, extended electronic states related to the highest occupied molecular orbital (HOMO) are formed within adenine and guanine stacks. The measurements provide clear evidence for a significant parallel dispersion of several HOMO-derived bands along quasi-one-dimensional stacks formed by π - π stacking in the direction normal to the surface. The dispersions can be traced over several periods and indicate a repeat unit of two molecules for guanine [1] and four molecules for adenine [2]. The band width of about 331 ± 8 meV for guanine and of 160 ± 30 meV for adenine and a very small effective mass of a positive charge carrier in both cases suggest the occurrence of band-like charge transport and a high but anisotropic hole mobility (>18 cm²/(V s)) at room temperature.

References

- [1] R. Friedlein, Y. Wang, A. Fleurence, F. Bussolotti, Y. Ogata, Y. Yamada-Takamura, J. Am. Chem. Soc. 132, 12808 (2010).
- [2] Y. Wang, A. Fleurence, Y. Yamada-Takamura, R. Friedlein, submitted.

10-2A

Fabrication of highly ordered organic biradical molecular film

Kaname Kanai¹, Hiroyuki Yoshida², Rie Suizu³, Masayuki Chikamatsu⁴, Takashi Kubo⁵, Kunio Awaga³, Naoki Sato², Masashi Nakatake⁶, Kazuhiro Nakasuji⁷

¹ *Department of Physics, Faculty of Science and Technology, Tokyo University of Science*

² *Institute for Chemical Research, Kyoto University*

³ *Department of Chemistry, Graduate School of Science, Nagoya University*

⁴ *Photonics Research Institute, National Institute of Advanced Industrial Science and Technology*

⁵ *Department of Chemistry, Graduate School of Science, Osaka University*

⁶ *HiSOR, Hiroshima University*

⁷ *Fukui University of Technology*

E-mail: kaname@ph.noda.tus.ac.jp

Most work in the field of organic electronics has focused on closed-shell molecules, and less attention has been paid to molecules with unpaired electrons in spite of their possibility. However, it has been reported that some stable organic radicals exhibit semiconducting properties and have smaller energy gaps than closed-shell organic semiconductors. Semiconducting organic radicals will be recognized as a potentially new class of materials for organic electronics, which becomes new building blocks for semiconducting layer in the devices. A device made from such a material is expected to have notably different operating principles in comparison with conventional devices. On the other hand, the fabrication of the highly ordered structure on their solid film is desired in order to take advantage of their unusual properties for the realization of new functions.

In this work we present studies on two different types of organic biradicals: first, thiazyl diradical, 4,4'-bis(1,2,3,5-dithiadiazolyl) (BDTDA) and second, diphenyl derivative of *s*-indacenodiphenalene (Ph₂-IDPL). BDTDA forms a stable dimer and which strongly interacts with each other and they develop a three-dimensional network in the solid film. We present a direct observation of the energy band structure of well-ordered BDTDA thin film probed by angle-resolved ultraviolet photoemission spectroscopy (ARUPS). It was found that BDTDA dimers formed highly crystalized film showing small and wide energy dispersions in the directions along parallel and perpendicular to the substrate, respectively.

Ph₂-IDPL is a unique biradical species that is hydrocarbon and possesses a small HOMO-LUMO gap and quite strong intermolecular interactions. It was found that the gas-deposition method substantially improved crystallinity of the film. Ph₂-IDPL molecules form a quasi one-dimensional molecular array normal to the substrate surface in the obtained film. The enhancement of the crystallinity dramatically improved ambipolar field effect properties of the Ph₂-IDPL film. In this talk, a relation between the electronic structure by the electric properties are also discussed.

Electronic structures of organic semiconductors studied by photoelectron yield spectroscopy: From single crystal to liquid sample

H. Ishii^{1,2}, H. Kinjo², T. Yamashita², Y. Noguchi^{1,2}, and Y. Nakayama¹

¹Center for Frontier Science, Chiba University

²Graduate School of Advanced Integration Science, Chiba University

E-mail: ishii130@faculty.chiba-u.jp

The information of the electronic structures of organic electronic materials is indispensable for understanding and improving organic electronics. So far, photoelectron spectroscopy (PES) has been widely applied for that purpose. In order to investigate practical electronic structure, PES is often not available due to sample charging and measurement environment problems. To overcome those, we have focused on photoelectron yield spectroscopy (PYS). By using current-mode-detection of photoelectron, PYS can be performed both in vacuum and atmospheric condition. By applying an electric field to sample surface, we can measure PYS even for extremely insulating materials [1]. In this paper, we will report on recent efforts of PYS investigation of electronic structures of various materials in practical situation that cannot be studied by conventional PES. The main topics are as follows: (i) The electronic structure of anthracene single crystal, especially, on the sublimation-induced change of surface structure and electronic structure, (ii) The electronic structures of liquid organic semiconductors, especially, 9-(2-ethylhexyl)carbazole (EHCz) liquid, which has attracted much attention in relation to an organic light emitting diode using liquid organic semiconductor.

References

[1] Y. Nakayama et al., Appl. Phys. Lett. 92 (2008) 153306 and 93(17) (2008) 173305.

ABSTRACTS FOR POSTER PRESENTATIONS

First-principles study on spin-polarized electric current in C/BN hetero-nanotubes

Huy Duy Nguyen and Tomoya Ono

Department of Precision Science and Technology, Graduate School of Engineering, Osaka University, 2-1 Yamada-oka, Suita, Osaka 565-0871, Japan

Email: huy@cp.prec.eng.osaka-u.ac.jp

Carbon nanotubes (CNT) are attracting lots of attention due to their high carrier mobility and low-intrinsic spin-orbit interaction. Other elements such as B and N are often utilized along with C enriching the electronic properties. However, in these nano-materials, the electronic reconstruction at the boundaries, i.e. edge state [1-4], is also important in determining the electronic structures of the whole systems. We investigate the (9,0) C/BN hetero-nanotubes, of alternative placement, for the magnetic behavior of edge states and the electron-transport properties.

The density functional theory calculations show that localized electronic states (edge states) appear at interfaces of C/BN hetero-nanotubes, as a result of CNT finite length. Due to the potential difference between B and N sites, these edge states are split into occupied and unoccupied states dominating density of states at the Fermi level. Thus doping which takes electrons (holes) from the edge states could induce magnetization. We adopt substitutional doping which replaces one C atom by one B atom at a C-N bond and find that it is in some sense analogous to the carrier doping, in which the electronic structure is spin-polarized. By sandwiching doped nanotubes between jellium electrodes, see Fig. 1, spin-polarized electronic current is realized.

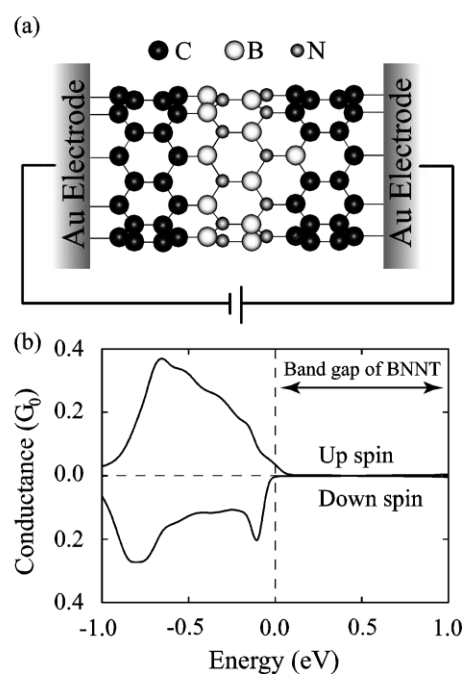


FIG. 1. B-doped $C_4(BN)_2$ nanotube is sandwiched between gold jellium electrodes (a) and plot of conductance versus the electron incident energy (b). The Fermi level is taken to be zero.

References

- [1] M. Fujita, K. Wakabayashi, K. Nakada, and K. Kusakabe, *J. Phys. Soc. Jpn.* **65**, 1920 (1996).
- [2] K. Wakabayashi, M. Fujita, H. Ajiki, and M. Sigrist, *Phys. Rev. B* **59**, 8271 (1999).
- [3] S. Okada, M. Igami, K. Nakada, and A. Oshiyama, *Phys. Rev. B* **62**, 9896 (2000).
- [4] J. Choi, Y. H. Kim, K. J. Chang, and D. Tománek, *Phys. Rev. B* **67**, 125421 (2003).

Electron-electron correlation energy calculations by superposition of non-orthogonal Slater determinants

Akira Sasaki, Kikuji Hirose and Hidekazu Goto

*Department of Precision Science & Technology, Graduate School of Engineering, Osaka University,
2-1 Yamada oka, Suita, Osaka 565-0871, Japan*

E-mail: a-sasaki@cp.prec.eng.osaka-u.ac.jp

A simple and practical scheme for calculations of electronic structures in few-electron systems with non-orthogonal basis set is presented [1-3]. The accuracy and applicability of the proposed scheme is demonstrated through calculations for the electronic structures of groundstates of atoms and molecules. As a many-electron wave function, a linear combination of Slater determinants (SDs) is employed. The one-electron wavefunction is constructed by a linear combination of Gaussian basis functions. The initial wavefunction is arranged by using the Hartree-Fock (HF) solutions, and the i th one-electron wavefunction in the A th SD is updated by taking linear independent N_c correlation functions. Thus we have a linear combination of $L+N_c$ SDs as N -electron wavefunctions and the expansion coefficients are given by the variational principle with respect to the total energy. Here, L represents the number of SDs. Iteration of this update leads the wavefunction to the groundstate by superposition of non-orthogonal SDs. Total energy convergence of carbon atom with 6-31G* basis set is demonstrated and the groundstate of carbon atom is obtained by less than 100 non-orthogonal SDs with an error of 0.003%. On the contrary, full configuration interaction (CI) requires over 10^5 orthogonalized SDs. The number of SDs required for the groundstates gradually increases with the present method although the ones with full CI increase explosively. Energy convergence depending on the number of correction vectors N_c is presented for Be atom. The convergence performance is improved by increasing the number of N_c . The present method can calculate essentially exact groundstate energies for few-electron systems. Calculations employing periodic boundary conditions and pseudopotentials will be made in a future study.

References

- [1] H. Goto and K. Hirose, *J. Phys.: Condens. Matter* 21, 064231 (2009).
- [2] H. Goto, K. Hirose, et al., *J. Comput. Theor. Nanosci.* 6, 2576 (2009).
- [3] H. Goto and K. Hirose, *J. Nanosci. Nanotechnol.* 11, 2997 (2011).

Desorption behaviors of alkanethiol self-assembled monolayers studied by thermal desorption spectroscopy

Eisuke Ito¹, Hungu Kang², Youyong Kim², Hiromi Ito¹, Tomohiro Hayashi³, Jaegeun Noh², Masahiko Hara^{1,3}

¹*Flucto-Order Functions Research Team, RIKEN-HYU Collaboration Center, RIKEN-ASI, 2-1 Hirosawa, Wako, Saitama 351-0198*

²*Department of Chemistry, Hanyang University, 17 Haendang-dong, Seondong-gu, Seoul 133-791, Korea*

³*Department of Electronic Chemistry, Tokyo Institute of Technology, 4259 Nagatuta, Midori-ku, Yokohama 226-8502, Japan*

E-mail: eito@riken.jp

We have been investigating thermal desorption processes of S-contained organic molecules in self-assembled monolayers (SAMs) on Au(111) using thermal desorption spectroscopy (TDS) [1]. From desorption temperature and detection of mass fragments in TDS spectra, adsorbed species, adsorption energy, and thermal stability can be estimated. TDS is a powerful method for examining adsorption states and thermal stability of SAMs. Here, we will summarize our TDS results of SAMs.

- A. We are interested in desorption process of alkanethiol SAMs. Usually, three kinds of fragments are observed in a TDS spectrum of an alkanethiol SAM on Au. At first, dimer fragments are observed at about 400 K, showing formation of disulfides on Au surface. And then, two fragments, thiols and thiolates are observed at the higher temperature. The desorption intensities and peak temperatures of these fragments depends on molecular structures, molecular density, and metal surfaces. We will show (i) the desorption properties of alkanethiol SAMs on Au, Ag, and Cu, and (ii) steric effect of desorption process.
- B. Adsorbed species can be identified by TDS experiments. This confirms molecular adsorption without decomposition. For examples, we concluded that fluorinated benzenethiols are adsorbed on Au(111) without scission of C-F and C-S bonds. Recently, we examined exchange process of adamantanethiol (AMT) and cyclohexanethiol (CHT) in a SAM. These molecules have different masses each other, and we can distinguish adsorption of these molecules. Exchange of AMT in CHT SAM was observed, while no CHT was inserted in AMT SAM.

References

[1] (a)H. Kang, et al., *Langmuir* **26**, 2983 (2010); (b)J. Noh, E. Ito, M. Hara, *J. Colloid Inter. Sci.* **342**, 513 (2011); (c)T. Hayashi et al., *J. Phys. Chem. C* **113**, 18795 (2009); (d)E. Ito, J. Noh, and M. Hara, *Surf. Sci.* **602**, 3291 (2008); (e)E. Ito, J. Noh, and M. Hara, *Chem. Phys. Lett.* **462**, 209 (2008); (f)E. Ito, J. Noh, and M. Hara, *Jpn. J. Appl. Phys.* **42**, L852 (2003).

Giant surface potential due to spontaneous noncentrosymmetric molecular orientation in vacuum-deposited thin film of Alq₃ derivatives

Takashi ISOSHIMA¹, Eisuke ITO¹, Youichi OKABAYASHI¹, Whee Won CHIN²,
Jin Wook HAN², Masahiko HARA¹

¹*Flucto-Order Functions Research Team, RIKEN-HYU Collaboration Research Center, RIKEN
Advanced Science Institute, Japan*

²*Department of Chemistry, Hanyang University, Korea*

E-mail: isoshima@riken.jp

Tris(8-hydroxyquinolinato) aluminum (III) (Alq₃) and similar ML₃-type compounds (M: metal, L: organic ligand) are organic semiconductors popularly used in various organic devices. These materials are often employed as vacuum-deposited thin films. Molecular orientation in the film is important since it affects optical and electric properties. Alq₃ and ML₃-type materials are known to present spontaneous huge surface potential when vacuum-deposited in dark [1]. The surface potential is linearly proportional to the film thickness as large as 50 V/μm, hence called giant surface potential (gSP). gSP originates from polar (noncentrosymmetric) molecular orientation in the amorphous thin films. It is also known that gSP reduces by irradiation of visible light. In this presentation, we describe our investigation on the spontaneous polar molecular orientation and gSP phenomenon in Alq₃ and related materials.

Polar molecular orientation can be investigated through 2nd-order nonlinear optical measurement. We employed the 1st-order electroabsorption (EA) spectroscopy. The order parameter of molecular orientation was evaluated to be *ca.* 0.01 even after photoinduced reduction of gSP, indicating that the reduction originates from electrostatic screening by photocarrier. We investigated dependence of gSP and molecular orientation on deposition conditions and on substrate materials, but the dependence was small. This suggests that interfacial interaction is not a critical factor to determine the molecular orientation. On the other hand, we found that chemical structure of the molecule significantly affects gSP and polar molecular orientation. Peripherally substituted Al(5-Clq)₃ presented about twice as high gSP, and Al(7-Prq)₃ (Pr=propyl) presented *negative* gSP. These results suggest controllability of magnitude and polarity of gSP and molecular orientation by chemical modification. These facts are important in terms of elucidation for spontaneous molecular orientation and also interesting in applications, enabling us to control interfacial electronic properties and nonlinear optical properties.

References

[1] E. Ito, Y. Washizu, N. Hayashi, H. Ishii, N. Matsuie, K. Tsuboi, Y. Ouchi, Y. Harima, K. Yamashita, and K. Seki, *J. Appl. Phys.*, **92**, 7306 (2002).

Correlation between energy level alignment and device performance in small-molecule based organic photovoltaic cells

Kouki Akaike^{1,2}, Yoshihiro Kubozono¹

¹Graduate School of Science and Technology, Okayama University

²Photoelectric Conversion Research Team, Advanced Science Institute, RIKEN

E-mail: akaike@riken.jp

Interfaces in organic photovoltaics (OPVs) are critical in determining effective charge generation and extraction. Recently, influence of substrate work function on electronic structure at organic/organic interfaces has been reported [1-3]. These studies indicate that OPV-structured specimen, which includes buffer layer and cathode metal, is necessary for deep understanding of carrier energetics and device performances of OPVs. Here, we have investigated the energy level alignment in small-molecule based OPVs: indium tin oxide (ITO)/copper phthalocyanine (CuPc)/fullerene (C₆₀)/bathocuproine (BCP)/Al cells, using Kelvin probe (KP) method. It was found that four events take place in the device; (1) downward energy shift at ITO/CuPc interface, (2) two-steps energy shifts at CuPc/C₆₀ interface, (3) large downward energy shift at C₆₀/BCP interface and (4) upward energy shift at BCP/Al interface [4]. Besides, we fabricated an OPV cell on an ITO substrate with low-work function to know the influence of substrate work function on the energy level alignment at each interface. The large built-in-potential at CuPc/C₆₀ interface is induced by employing low-work, while electronic structures at C₆₀/BCP/Al interfaces are not modified by the substrate work function [4]. Photocurrent in the latter OPV cell is significantly suppressed, and short circuit current is nulled. Comparing current density – voltage characteristics and electronic structure in two OPVs, electronic structure at CuPc/C₆₀ interface is quite important for effective carrier generation and transport. In presentation, KP measurements on other OPV cells will be also reported.

References

- [1] J. X. Tang, C. S. Lee, and S. T. Lee, *J. Appl. Phys.* **10**, 064504 (2007).
- [2] S. Braun, M. P. de Jong, W. Osikowicz, and W. R. Salaneck, *Appl. Phys. Lett.* **91**, 202108 (2007).
- [3] W. Zhao, E. Salomon, Q. Zhang, S. Barlow, S. R. Marder, and A. Kahn, *Phys. Rev. B*, **77**, 165336 (2008).
- [4] K. Akaike and Y. Kubozono, in preparation.

P-6

Study on the electronic properties of C₆₀ and bathocuproine interface using ultraviolet photoelectron spectroscopy

S. Wang¹, T. Sakurai^{1,2}, R. Kuroda¹, S. Toyoshima¹, H. Kato³, K. Akimoto¹

¹ Institute of Applied Physics, University of Tsukuba, Tsukuba, Ibaraki 305-8573, Japan

² PRESTO, Japan Science and Technology Agency (JST), Kawaguchi, Saitama 332-0012, Japan

³ Graduate School of Science and Technology, Hirosaki University, Hirosaki, Aomori 036-8561, Japan

E-mail: wsh8511@gmail.com

Based on the enhancement effect of bathocuproine (BCP) insertion layer between C₆₀ and metal anode to the efficiency of organic solar cells (OSC) and the ambiguity of physical mechanism, the interfacial electronic properties of metal/BCP/C₆₀ interfaces were studied by ultraviolet photoelectron spectroscopy (UPS). The results showed that the highest occupied molecular orbital (HOMO) of BCP was independent on the work function of metal, indicating the Fermi energy pinning [1]. After depositing C₆₀ layer with high coverage on BCP, presenting bulk C₆₀, the HOMO of C₆₀ downshifted. Fig.1 showed the HOMO of C₆₀ dependence on BCP thickness deposited on Ag or Ca substrate. The HOMO of C₆₀ showed downward shift gradually at initial BCP coverage, and then shifted abruptly much deeper. The corresponding BCP thicknesses for this steep evolution are 0.8 nm and 1.6 nm for Ag and Ca substrate, respectively, which is coincided with the change of gap states at metal/BCP interfaces. The evolution of C₆₀ HOMO may be caused by the induced gap states or the diffusion of metal atoms to C₆₀ layer.

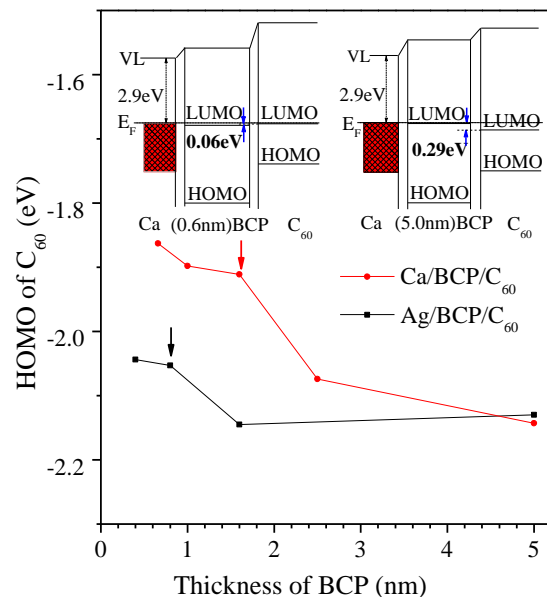


Fig.1 the HOMO of C₆₀ dependence of BCP thickness and the energy level alignment of Ca/BCP/C₆₀

The inset of Fig.1 showed the energy level diagram of Ca/BCP/C₆₀. The energy difference of lowest unoccupied molecular orbital (LUMO) between BCP and C₆₀ are 0.06 eV and 0.29 eV for 0.6 nm BCP and 5.0 nm BCP, respectively. The electron barrier exists between C₆₀ and BCP in the thick BCP case while LUMO nearly coincides with each other when BCP layer is thin, being in agreement with the results of the performances of solar cells with various thickness BCP [2]. It can be concluded that the energy level alignment of OSC interfaces is greatly dependence on BCP thickness and Ca can lower the barrier of BCP/C₆₀ interface.

References

- [1] S. Sakurai, et al., J. Appl. Phys., **107**, 043707 (2010).
- [2] C. Chang, et al., Appl. Phys. Lett., **96**, 263506 (2010).

Characterization of an organic thin film device under operational condition by fluorescence-yield X-ray absorption spectroscopy

H. S. Kato^{1,†}, H. Yamane², N. Kosugi², M. Kawai^{1,3}

¹ Advanced Science Institute, RIKEN, Wako, Saitama, Japan

² Institute for Molecular Science (IMS), Okazaki, Aichi, Japan

³ Department of Advanced Materials Science, University of Tokyo, Kashiwa, Chiba, Japan

[†] Present Affiliation: Department of Chemistry, Osaka University, Toyonaka, Osaka, Japan

E-mail: hirokato@chem.sci.osaka-u.ac.jp

In order to develop well designed molecular devices, it is desired to observe *in situ* electronic states under operational condition. In this study, we aim to elucidate the electronic state of organic thin film transistors (OTFTs) by the fluorescence-yield X-ray absorption spectroscopy (FY-XAS), which should be a promising method for detection of electronic states of inner organic thin film devices, because the fluorescent X-rays have a long penetration depth of about 100 nm in most of materials even for the soft X-ray region and are not disturbed by applied electric fields [1,2].

To investigate the electronic states of OTFT, α,ω -dihexylsexithiophene (DH6T) thin films on the SiO₂-covered Si substrates were fabricated. The FY-XAS measurements were performed at the BL3U beamline of the UVSOR facility in IMS. The fluorescence intensities were measured using a retarding field detector consisting of the MCP system.

The element-specific observation of electronic states of DH6T films even beneath Au electrodes was achieved [2]. The molecular orientation in the Au-deposited films was clearly confirmed by the C K-edge FY-XAS measurements. In addition, the bias dependence of the FY-XAS spectra of DH6T films was successfully detected (Fig. 1), in which the origin of the spectral change was considered to be a molecular state modification by the applied electric field. The feature of difference spectra in the bias dependence suggested that the applied electric field is not uniform in the DH6T films. This method has many advantages to observe the inner part of heterogeneous thin films and thus will be utilized for characterizing various organic thin film devices.

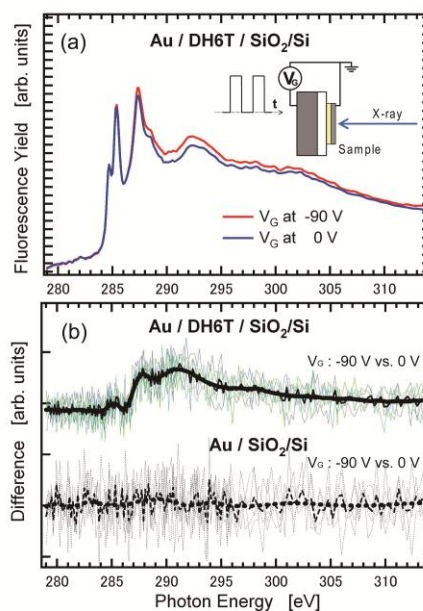


Fig. 1 Bias dependence of the C K-edge FY-XAS spectra of the Au-covered DH6T films (17 nm thick) measured at normal incidence geometry: (a) the spectra at the biases of 0 V and -90 V, (b) spectral changes at the biases from 0 V to -90 V (solid lines) as compared with that of a DH6T-lacked sample (broken lines).

References

- [1] H.S. Kato *et al.*, J. Electron Spectrosc. Relat. Phenom. **174**, 93 (2009).
- [2] H.S. Kato, H. Yamane, N. Kosugi, M. Kawai, Phys. Rev. Lett. *in press* (2011).

Local and global electronic spectroscopy of unoccupied states: Naphthalene on HOPG studied by the combination of 2PPE and STM

T. Yamada, M. Isobe, M. Shibuta, H. S. Kato and T. Munakata

Department of Chemistry, Graduate School of Science, Osaka University, Toyonaka OSAKA 560-0043, Japan

E-mail: tyamada@chem.sci.osaka-u.ac.jp

We have investigated the correlation between adsorption geometries and their electronic structures by using low temperature Scanning Tunneling Microscope (STM) and Two-Photon Photoemission (2PPE) [1]. In 2PPE, femtosecond laser is used as a light source in order to detect occupied and unoccupied states in the vicinity of the Fermi level. In STM experiments, local tunneling spectroscopy (z-V spectroscopy) is performed by recording the tip-sample separations as a function of applied sample voltage with the constant current feedback engaged.

Naphthalene molecules adsorbed on HOPG is used as a model system. As shown in Fig.1, $(2\sqrt{3}\times 2\sqrt{3})R30^\circ$ and $(5\ 2, 2\ 3)$ superstructures are formed for sub-monolayer islands and multilayer films, respectively. In z-V spectroscopy, the first Image Potential States (IPS($n=1$)) are detected on all surfaces but at different energies. IPS is a quantized bound state derived from the Coulomb-like image potential on the vacuum side. Geometrical structure dependent shifts of IPS are also observed in 2PPE spectroscopy. In addition, unoccupied feature which is specific to the $(2\sqrt{3}\times 2\sqrt{3})R30^\circ$ island is observed. This feature can be assigned to the LUMO of the first layer, but disappears at multilayer film. This indicates a drastic change of electronic states occurs associated with the change of the geometric structure. It should be noted that all of unoccupied features are observed in 2PPE spectroscopy at energies shifted by 0.8 - 0.9 eV. These shifts can be ascribed to STM tip induced effect (Stark shift). Ranging from nano to micrometer scale, we can clarify one-to-one link between geometric and electronic structures.

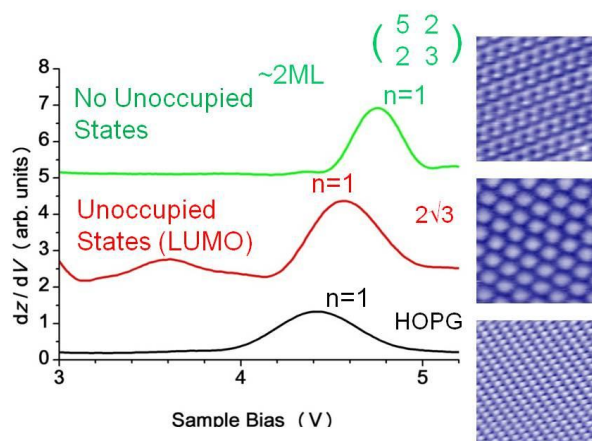


Fig. 1 z-V spectra obtained on the corresponding STM images (right, 5.4nm^2). Clean HOPG, $(2\sqrt{3}\times 2\sqrt{3})R30^\circ$ for sub monolayer, and $(5\ 2, 2\ 3)$ for multilayer are shown from bottom to top.

References

[1] T. Yamada, M. Shibuta, Y. Ami, Y. Takano, A. Nonaka, K. Miyakubo and T. Munakata J. Phys. Chem. C, 114, 13334 (2010).

Experimental study of epitaxial silicene on zirconium diboride

Antoine Fleurence, Rainer Friedlein, Taisuke Ozaki, Ying Wang and Yukiko Yamada-Takamura

School of Materials Science, Japan Advanced Institute of Science and Technology, 1-1 Asahidai, Nomi, Ishikawa 923-1292, Japan,
E-mail: antoine@jaist.ac.jp

Since its electronic properties are predicted to be similar to those of graphene [1], silicene, the silicon counterpart to graphene, has recently attracted a lot of attention. It may challenge graphene in electronic devices since its integration into already existing silicon-based microelectronics might be easier to be accomplished. Theoretical calculations predict the existence of a stable, slightly buckled structure similar to that of a Si(111) monolayer [1]. So far, there are only a few experimental observations of two-dimensional silicene. Its properties have been well characterized only while being in the form of one-dimensional ribbons formed on Ag(110) [2].

In the present work, using scanning tunneling microscopy (STM), surface-sensitive core-level and angle-resolved ultraviolet photoelectron spectroscopy (ARUPS), we provide evidence for the spontaneous formation of two-dimensional silicene layers on the surface of (0001)-oriented ZrB₂ thin films grown on Si(111). The highly-resolved STM images indicate the presence of a honeycomb lattice with a lattice parameter that is 5 % smaller than that of bulk Si(111). The ($\sqrt{3}\times\sqrt{3}$)-reconstructed silicene layer exhibits a commensurate relationship to the (2x2) unit cell of ZrB₂(0001). As a consequence, the silicon layer appears as a (2x2) reconstruction of the ZrB₂(0001) surface.

Si 2*p* photoelectron spectra recorded using a photon energy of 130 eV demonstrates unambiguously the presence of three distinct chemical states of the Si atoms supporting the structure model. Moreover, clear differences in photoelectron diffraction patterns taken along the ZrB₂[11-20] and ZrB₂[1-100] directions confirm the buckling of the silicene layer.

At larger length scale, the silicene layer is textured into a superstructure made of a one-dimensional array of reconstructed domains [3] allowing the release of surface stress. Strong evidence for the two-dimensional nature of the silicene layer is found in the band structure determined by ARUPS. Our finding is therefore a clear experimental evidence for the stability of a graphene-like, two-dimensional crystal made of silicon atoms.

References

- [1] S. Cahangirov, *et al.*, Phys. Rev. Lett. **102**, 236804 (2009).
- [2] P. De Padova, *et al.*, Appl. Phys. Lett. **96**, 261905 (2010).
- [3] Y. Yamada-Takamura, *et al.*, Appl. Phys. Lett. **97**, 073109 (2010).

P-10

van der Waals density functional applied to adsorption systems

Ikutaro Hamada

WPI-Advanced Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan
E-mail: ikutaro@wpi-aimr.tohoku.ac.jp

The van der Waals interaction plays an important role in weakly interacting organic crystals and organic/metal interfaces. However, conventional density-functional theory with local and semilocal approximations is known to describe the van der Waals interaction very poorly. Here I report recent progress in the van der Waals density functional theory[1], a promising density functional which accounts for the van der Waals interaction within the framework of density-functional theory. I show by using appropriate exchange and nonlocal correlation energy functionals, it is possible to describe geometries and electronic structures of organic/metal interfaces accurately. Feasibility of the improved version of vdW-DF is illustrated by its application to graphene/metal[2] and fullerene/metal[3] interfaces.

References

- [1] M. Dion, H. Rydberg, E. Schröder, D. C. Langreth, and B. I. Lundqvist, *Phys. Rev. Lett.* **92**, 246401 (2004).
- [2] I. Hamada and M. Otani, *Phys. Rev. B* **82**, 153412 (2010).
- [3] I. Hamada and M. Tsukada, *Phys. Rev. B* **83**, 245437 (2011).

First-principles study of CO oxidation on carbon alloy catalysts

Shintaro Iseki, Kouji Inagaki, Yoshitada Morikawa

*Department of Precision Science and Technology, Graduate School of Engineering, Osaka University,
2-1 Yamada oka, Suita, Osaka 565-0871, Japan*

E-mail: iseki@cp.prec.eng.osaka-u.ac.jp

Recently, several researchers reported surprisingly high oxygen reduction reaction activity in carbon-based nanomaterials doped with N and B [1]. It has been attracting a growing interest as potential Pt-free oxygen reduction catalysts for polymer electrolyte fuel cells as well as for CO oxidation catalysts. There are two basic shapes for graphene sheet edges, namely, armchair and zigzag edges. The zigzag edge has localized electronic states and a sharp peak appears in the density of states near the Fermi level. Ikeda and co-workers revealed that the oxygen adsorption and reduction reactions are enhanced if graphite-like N and B atoms are located near zigzag edges [2,3]. In this research, we investigate oxidation processes of CO on carbon alloy catalysts by using first principles calculations. We used a program package “STATE” (Simulation Tool for Atom TEchnology) [4], which is based on density functional theory within a generalized gradient approximation with a plane wave basis set and ultrasoft pseudopotentials. We employed a repeated slab model and one unit cell consists of four graphene sheets with 48 C atoms. C atom near a zigzag edge is replaced with a N or B atom. An O₂ molecule is adsorbed at the zigzag edge and we investigated CO oxidation by the adsorbed O₂ molecule. Activation barriers for CO oxidation processes were estimated by the Climbing Image Nudged Elastic Band method [5] and we obtained the activation barrier of about 8kJ/mol. It is much lower than that of CO oxidation on Pt surfaces. In the poster presentation, we will discuss the electronic structure of N and B doped graphite edges and their relation to CO oxidation processes.

References

- [1] J. Ozaki, N. Kimura, T. Anahara, A. Oya, *Carbon*, **45** 1847 (2007).
- [2] T. Ikeda, M. Boero, S. Huang, K. Terakura, M. Oshima, J. Ozaki, *J. Phys. Chem. C*, **112**, 14706 (2008).
- [3] T. Ikeda, M. Boero, S. Huang, K. Terakura, M. Oshima, J. Ozaki, S. Miyata *J. Phys. Chem. C*, **114**, 8933 (2010).
- [4] Y. Morikawa, *Phys. Rev. B* **63**, 033405 (2001).
- [5] G. Henkelman, B. P. Uberuaga, and H. Jonsson, *J. Chem. Phys.* **113**, 9901 (2000).

PARTICIPANTS LIST

Name	Affiliation	E-mail Address
Akaike, Kouki	Photoelectric Conversion Research Team RIKEN	akaike@riken.jp
Bussolotti, Fabio	Graduate School of Advanced Integration Science, Chiba University	fabio@restaff.chiba-u.jp
Coropceanu, Veaceslav	Center for Organic Photonics and Electronics and School of Chemistry and Biochemistry, Georgia Institute of Technology	coropceanu@gatech.edu
Crispin, Xavier	Linköping University Department of Science and Technology	xavcr@itn.liu.se
Duhm, Steffen	Graduate School of Advanced Integration Science	duhm@restaff.chiba-u.jp
Fahlman, Mats	Department of Physics, Chemistry and Biology, Linköping University	mafah@ifm.liu.se
Fleurence, Antoine	School of Materials Science, Japan Advanced Institute of Science and Technology	antoine@jaist.ac.jp
Friedlein, Rainer	School of Materials Science, Japan Advanced Institute of Science and Technology	friedl@jaist.ac.jp
Fujikawa, Takashi	Graduate School of Advanced Integration of Science, Chiba University	tfujikawa@faculty.chiba-u.jp
Goto, Hidekazu	Department of Precision Science & Technology, Osaka University	goto@prec.eng.osaka-u.ac.jp
Hamada, Ikutaro	WPI-Advanced Institute for Materials Research, Tohoku University	ikutaro@wpi-aimr.tohoku.ac.jp
Hirose, Kenji	Green Innovation Research Laboratories, NEC Corporation	hirose@kbd.biglobe.ne.jp
Inagaki, Kouji	Department of Precision Science and Technology & Applied Physics, Graduate School of Engineering, Osaka University	inagaki@prec.eng.osaka-u.ac.jp
Iseki, Shintaro	Precision Science and Technology, Graduate School of Engineering, Osaka University	iseki@cp.prec.eng.osaka-u.ac.jp
Ishii, Hisao	Center for Frontier Science, Chiba University	ishii130@faculty.chiba-u.jp
Isoshima, Takashi	Flucto-Order Functions Research Team, RIKEN-HYU Collaboration Research Center, RIKEN Advanced Science Institute	isoshima@riken.jp
Ito, Eisuke	Flucto-Order Functions Research Team, RIKEN	eito@riken.jp
Kanai, Kaname	Dept. Physics, Tokyo University of Science	kaname@ph.noda.tus.ac.jp
Kato, Hiroyuki S.	Department of Chemistry, Graduate School of Science, Osaka University	hirokato@chem.sci.osaka-u.ac.jp
Kera, Satoshi	Graduate School of Advanced Integration Science, Chiba University	kera@faculty.chiba-u.jp
Koch, Norbert	Institut für Physik, Humboldt-Universität zu Berlin	norbert.koch@physik.hu-berlin.de
Kumpf, Christian	Peter Grünberg Institute (PGI-3) Forschungszentrum Jülich	c.kumpf@fz-juelich.de
Liu, Xianjie	Department of Physics, Chemistry and Biology Linköping University	xjliu@ifm.liu.se
Morikawa, Yoshitada	Department of Precision Science and Technology, Graduate School of Engineering, Osaka University	morikawa@prec.eng.osaka-u.ac.jp

Name	Affiliation	E-mail Address
Munakata, Toshiaki	Department of Chemistry, Graduate School of Science, Osaka University	munakata@ch.wani.osaka-u.ac.jp
Murdey, Richard	Institute for Chemical Research, Kyoto University	rmurdey@e.kuicr.kyoto-u.ac.jp
Nakayama, Yasuo	Center for Frontier Science, Chiba University	nkym@restaff.chiba-u.jp
Nguyen, Huy Duy	Precision Science and Technology, Graduate School of Engineering, Osaka University	huy@cp.prec.eng.osaka-u.ac.jp
Ono, Tomoya	Research center for Ultra-Precision Science and Technology, Graduate School of Engineering, Osaka University	ono@prec.eng.osaka-u.ac.jp
Sakamoto, Kazuyuki	Department of Nanomaterials Science, Chiba University	kazuyuki_sakamoto@faculty.chiba-u.jp
Sakurai, Takeaki	Institute of Applied Physics, University of Tsukuba	sakurai@bk.tsukuba.ac.jp
Salaneck, William R.	Department of Physics, Chemistry and Biology, Linköping University	william.r.salaneck@liu.se
Sasaki, Akira	Precision Science and Technology, Graduate School of Engineering, Osaka University	a-sasaki@cp.prec.eng.osaka-u.ac.jp
Siegbahn, Hans	Department of Physics and Astronomy, Uppsala University	hans.siegbahn@fysik.uu.se
Söderström, Johan	Department of Physics and Astronomy, Uppsala University	johan.soderstrom@physics.uu.se
Ueno, Nobuo	Department of Nanomaterial Science, Graduate School of Advanced Integration Science, Chiba University	uenon@faculty.chiba-u.jp
Vollmer, Antje	Helmholtz Zentrum Berlin f. Materialien und Energie GmbH, Synchrotron Storage Ring BESSY II	antje.vollmer@helmholtz-berlin.de
Wang, Shenghao	Institute of Applied Physics, University of Tsukuba	wsh8511@gmail.com
Wang, Ying	School of Material Science, Japan Advanced Institute of Science and Technology	wang-y@jaist.ac.jp
Yamada, Takashi	Department of Chemistry, Graduate School of Science, Osaka University	tyamada@chem.sci.osaka-u.ac.jp
Yamada-Takamura, Yukiko	School of Material Science, Japan Advanced Institute of Science and Technology	yukikoyt@jaist.ac.jp
Yamamoto, Masayuki	Graduate School of Advanced Integration Science, Chiba University	myamamoto@graduate.chiba-u.jp
Yamane, Hiroyuki	Dept. of Photo-Molecular Science, Institute for Molecular Science	yamane@ims.ac.jp
Yanagisawa, Susumu	Department of Physics and Earth Sciences, Faculty of Science, University of Ryukyus	shou@phys.u-ryukyu.ac.jp
Yoshida, Hiroyuki	Institute for Chemical Research, Kyoto University	yoshida@e.kuicr.kyoto-u.ac.jp
Yoshinobu, Jun	The Institute for Solid State Physics, The University of Tokyo	yoshinobu@issp.u-tokyo.ac.jp



Global COE, Chiba Univ.



Kaga City



VG SCIENTA
a gammatdata company



ADCAP VACUUM TECHNOLOGY



GEN-TECH, INC.

Vacuum & nano technology

分光計器

BUNKOHKEIKI Co., Ltd.