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Nov. 14, 2005 (Mon.)

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Opening (9:00 ~ 9:30)

Chair: S. Hasegawa (*Univ. of Tokyo*)

Plenary Session (9:30 ~ 11:50)

Chair: K. Takayanagi (*Tokyo Inst. of Tech.*)

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P. Avouris, *IBM T.J. Watson Research Center, USA* 1
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A. Fujishima, ¹ KAST and ² Central Japan Railway Company, Japan 2
- Chair: A. Ikai (*Tokyo Inst. of Tech.*)
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H.R. Sharma¹, M. Shimoda¹, V. Fournée², A.P. Tsai^{1,3} and A. Yamamoto¹,
¹ NIMS, Japan, ² CNRS, France and ³ Tohoku Univ., Japan 4
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F. Rose, S. Kawai, T. Ishii and H. Kawakatsu, *Univ. of Tokyo, Japan* 5
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Conference Room A

Session 1: Theoretical approaches to surface- and nano-structures and properties (9:00 ~ 12:50)

Chair: K. Shiraishi (*Univ. of Tsukuba*)

- 9:00 We-A1(I) Theory of dielectric and piezoelectric response in bulk materials and nanoscale superlattices
(Invited)
D. Vanderbilt, *Rutgers Univ., USA* 341
- 9:30 We-A2 First-Principles Study of Metal/Oxide Interfaces: Effects of Interface Stoichiometry
S. Tanaka¹, S. Shi¹, K. Okazaki^{1,2} and M. Kohyama¹, ¹ *AIST and* ² *JST-CREST, Japan* 342
- 9:45 We-A3 First-Principles Study of Organic/Metal Interfaces
R. Belkadi¹, Y. Shirakawa², M. Kohyama³, J. Hidaka² and S. Tanaka³,
¹ *JST, CREATE*, ² *Doshisha Univ. and* ³ *AIST, Japan* 343
- 10:00 We-A4 Periodic Density Functional Theory and Accelerated Quantum Chemical Molecular Dynamics
Study on Precious Metal/Oxide Interfaces
C.H. Jung¹, R. Ishimoto¹, H. Tsuboi¹, M. Koyama¹, A. Endou¹, M. Kubo^{1,2} and
A. Miyamoto¹, ¹ *Tohoku Univ. and* ² *PRESTO, JST, Japan* 344
- 10:15 We-A5 Molecular-dynamics simulations of thermal transport in carbon nanotubes with structural defects
N. Kondo^{1,2}, T. Yamamoto^{1,2} and K. Watanabe^{1,2},
¹ *Tokyo Univ. of Science and* ² *CREST, JST, Japan* 345
- 10:30 We-A6 Superlubricity of Graphite/C₆₀/Graphite Bearing System
N. Sasaki¹, N. Itamura¹, M. Ohyama² and K. Miura³, ¹ *Seikei Univ.*,
² *Univ. of Tsukuba and* ³ *Aichi Univ. of Education, Japan* 346

Break (10:45 ~ 11:05)

Chair: D. Vanderbilt (*Rutgers Univ.*)

- 11:05 We-A7 H segregation and Ag-cluster growth on the H-terminated Si(111) surface
H. Jeong and S. Jeong, *Chonbuk Nat. Univ., Korea* 347
- 11:20 We-A8 First-principles study of stair-rod dislocations in Si and GaAs stacking-fault tetrahedron defects
R. Kobayashi and T. Nakayama, *Chiba Univ., Japan* 348
- 11:35 We-A9(I) First-Principles Study of Self-Organization at N/Cu(001) Surface (Invited)
S. Tsuneyuki and Y. Yoshimoto, *Univ. of Tokyo, Japan* 349
- 12:05 We-A10 *Ab initio* energetics of phosphorus impurity in subsurface regions of hydrogenated diamond
surfaces
T. Miyazaki and S. Yamasaki, *AIST, Japan* 350
- 12:20 We-A11 Adsorption Properties of In and As on InAs(111)A surface
A. Taguchi¹ and K. Kanisawa¹, *NTT Basic Research Labs, Japan* 351
- 12:35 We-A12 Surface phase equilibria in MBE growth of strained In_{1-x}Ga_xAs heteroepitaxial layers
O. Chikalova-Luzina and N.N. Ledentsov, *Russian Academy of Sciences, Russia* 352

Conference Room B

Session 11: Surface chemistry and catalysis (9:00 ~ 10:45)

Chair: Y. Inoue (*Nagaoka Univ. of Tech.*)

- 9:00 We-B1 Surface Reactions of Co on SiO₂ thin layer/Si substrate Studied by LEEM and PEEM
F. Maeda¹, H. Hibino¹, S. Suzuki¹, Y. Kobayashi¹, Y. Watanabe² and F. Guo³,
¹ *NTT Basic Research Labs*, ² *NTT Advanced Technology Corp. and*
³ *The Japan Synchrotron Radiation Research Inst., Japan* 353
- 9:15 We-B2 Atomic-scale observation and control of the reaction of phosphine with silicon
S.R. Schofield¹, N.J. Curson², O. Warschkow³, N.A. Marks³, H.F. Wilson³,
M.Y. Simmons², P.V. Smith¹, M.W. Radny¹ and D.R. McKenzie³, ¹ *Univ. of Newcastle*,
² *Univ. of New South Wales and* ³ *Univ. of Sydney, Australia* 354

9:30	We-B3	Chemisorption of pyrazine and pyrrole on Si(001)-2×1: structural study by STM and PED M. Shimomura ¹ , D. Ichikawa ¹ , T. Kawaguchi ¹ , T. Abukawa ² , T. Aoyama ² , S. Kono ² and Y. Fukuda ¹ , ¹ <i>Shizuoka Univ. and</i> ² <i>Tohoku Univ., Japan</i> 355	355
9:45	We-B4	SAM of Surfactant on H-Terminated Si(111) Surfaces in Aqueous Solutions Studied by In-situ Measurements A. Imanishi ^{1,2} , R. Omoda ¹ , M. Suzuki ¹ and Y. Nakato ^{1,2} , ¹ <i>Osaka Univ. and</i> ² <i>CREST, JST, Japan</i> 356	356
10:00	We-B5	Ideal Methyl Termination of the Si(111) Surface T. Yamada ^{1,2} , M. Kawai ^{1,3} , A. Wawro ^{2,4} , S. Suto ² and A. Kasuya ² , ¹ <i>RIKEN</i> , ² <i>Tohoku Univ.</i> , ³ <i>Univ. of Tokyo, Japan and</i> ⁴ <i>Polish Academy of Sciences, Poland</i> 357	357
10:15	We-B6(I)	Chemical Modification of Semiconductor Surfaces: Basic Principles and Applications (Invited) S.F. Bent, <i>Stanford Univ., USA</i> 358	358

Session 7: Device applications of bio, metal, ceramics and hybrid, and organic films (11:05 ~ 12:50)

Chair: M. Nakamura (*Chiba Univ.*)

11:05	We-B7(I)	Separation, Trapping and Single Molecule Detection of DNA Employing Nanostructures (Invited) Y. Horiike, S. Hashioka, R. Ogawa and A. Oki, <i>NIMS, Japan</i> 359	359
11:35	We-B8	Uniaxial Alignment of Alq ₃ by Laser-Assisted Molecular Beam Epitaxy T. Shimada, T. Suzuki, T. Hasegawa, H. Ichikawa and K. Saiki, <i>Univ. of Tokyo, Japan</i> 360	360
11:50	We-B9	Pulsed laser patterning of organic transistor channel for interface characterizations K. Tsukagoshi ^{1,2} , J. Takeya ³ , I. Yagi ¹ , T. Takenobu ^{4,5} , Y. Iwasa ^{4,5} and Y. Aoyagi ^{1,6} , ¹ <i>RIKEN</i> , ² <i>PREST, JST</i> , ³ <i>CRIEPI</i> , ⁴ <i>Tohoku Univ.</i> , ⁵ <i>CREST, JST and</i> ⁶ <i>Tokyo Inst. of Tech., Japan</i> 361	361
12:05	We-B10	Nanoscale Molecular Transistor Fabrication using Self-Assembled Organic Multilayers T. Ishida ¹ , M. Nakano ² , M. Horikawa ¹ , H. Kuwahata ¹ , Y. Naitoh ¹ , K. Miyake ² and W. Mizutani ¹ , ¹ <i>NRI-AIST and</i> ² <i>AMRI-AIST, Japan</i> 362	362
12:20	We-B11(I)	Encoding and transport of information in molecular and biomolecular systems (Invited) J.M. Seminario, L. Yan and Y. Ma, <i>Texas A&M Univ., USA</i> 363	363

Auxiliary Hall C

Session 5: Self-assembly and self-organization for nanostructure formation, and characterization (9:00 ~ 12:50)

Chair: J. K. Kim (*POSTEC*)

9:00	We-C1	Close-packed Self-Assembled Monolayer (SAM) of Gold Nanoparticles: Fabrication, SERS and Near-field Spectroscopy M.K. Hossain ^{1,2} , K. Ishioka ^{1,2} , M. Kitajima ^{1,2} , K. Imura ³ and H. Okamoto ³ , ¹ <i>Univ. of Tsukuba</i> , ² <i>NIMS and</i> ³ <i>IMS, Japan</i> 364	364
9:15	We-C2	Temperature dependent film growth of DNA oligomers on mica S. Machida ^{1,2} , T. Nakayama ^{1,2,3} and M. Aono ^{1,2} , ¹ <i>ICRP, JST</i> , ² <i>NIMS and</i> ³ <i>Univ. of Tsukuba, Japan</i> 365	365
9:30	We-C3(I)	Directed assembly and characterization of organosilicon nanostructures using scanning tunneling microscopy (Invited) M.C. Hersam, <i>Northwestern Univ., USA</i> 366	366
10:00	We-C4	The Electronic Property and the Electrical Conductance of Polydiacetylene Molecules Y. Kuwahara ^{1,2,3} , M. Akai-Kasaya ² , T. Takami ¹ , A. Saito ^{1,2,3} and M. Aono ^{2,3,4} , ¹ <i>Osaka Univ.</i> , ² <i>ICORP, JST</i> , ³ <i>RIKEN and</i> ⁴ <i>NIMS, Japan</i> 367	367
10:15	We-C5	Aligned Growth of Isolated Single-Walled Carbon Nanotubes Programmed by Atomic Arrangement of Crystalline Surface H. Ago ^{1,2} , K. Nakamura ² , K. Ikeda ² , R. Ohdo ² , N. Uehara ² , M. Shinagawa ² , N. Ishigami ² and M. Tsuji ^{1,2} , ¹ <i>CREST-JST and</i> ² <i>Kyushu Univ., Japan</i> 368	368
10:30	We-C6	Robust one-dimensional metallic band structure of silicide nanowires H.W. Yeom, Y.K. Kim, E.Y. LEE, K.D. Ryang and P.G. Kang, <i>Yonsei Univ., Korea</i> 369	369

Break (10:45 ~ 11:05)

Chair: M.C. Hersam (*Northwestern Univ.*)

11:05	We-C7(I)	Nonlocal bond-angle manipulation by injected tunneling carriers on clean Ge(001) surface (Invited) F. Komori, Y. Takagi, Y. Yoshimoto and K. Nakatsuji, <i>Univ. of Tokyo, Japan</i> 370	370
11:35	We-C8	Low energy electron microscopy study of self-assembling Ge nanostructures on clean and Ga patterned Si(113) T. Clausen ¹ , Th. Schmidt ¹ , J.I. Flege ¹ , A. Locatelli ² , T.O. Menten ² , S. Heun ³ , F. Guo ⁴ and J. Falta ¹ , ¹ <i>Univ. of Bremen, Germany</i> , ² <i>Sincrotrone Trieste</i> , ³ <i>Lab. Nazionale TASC-INFN, Italy</i> and ⁴ <i>Spring-8/JASRI, Japan</i> 371	371
11:50	We-C9	Local electronic structure of Al nano-cluster fabricated on Si(111)7×7 surface H. Narita, M. Nakatake, T. Xie, T. Moko, A. Kimura, S. Qiao, H. Namatame and M. Taniguchi, <i>Hiroshima Univ., Japan</i> 372	372
12:05	We-C10	STM study of the structure BC ₃ sheet on NbB ₂ (0001) substrate A. Ueno ¹ , T. Fujita ¹ , M. Matsue ¹ , F. Patthey ² , H.-C. Ploight ² , W.-D. Schneider ² and C. Oshima ¹ , ¹ <i>Waseda Univ., Japan</i> and ² <i>École Polytechnique Fédérale de Lausanne, Switzerland</i> 373	373
12:20	We-C11	d-band broadening on Cu(100) due to the compressive strain D. Sekiba, Y. Yoshimoto, K. Nakatsuji and F. Komori, <i>Univ. of Tokyo, Japan</i> 374	374
12:35	We-C12	Self-organized formation of the ordered nanostructure arrays on Si surfaces V.G. Lifshits ¹ , A.A. Saranin ¹ , A.V. Zotov ¹ , M. Katayama ² and K. Oura ² , ¹ <i>Inst. of Autom. & Control Proc., Russia</i> and ² <i>Osaka Univ., Japan</i> 375	375

Conference Room A

Session 1: Theoretical approaches to surface- and nano-structures and properties (14:00 ~ 15:45)

Chair: S. Tsuneyuki (*Univ. of Tokyo*)

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14:15	We-A14	Electrical detection of chemical reactions on nano-space K. Yokota, M. Taniguchi and T. Kawai, <i>Osaka Univ., Japan</i> 377	377
14:30	We-A15	Tight-Binding Calculation of Electronic Conduction through Tamm Surface States Measured with Micro-Multi-Point STM Probes R. Suzuki ^{1,2} , M. Noda ^{1,2} , T. Tada ^{1,2} and S. Watanabe ^{1,2} , ¹ <i>Univ. of Tokyo</i> and ² <i>CREST, JST, Japan</i> 378	378
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15:00	We-A17	Ionization-Mediated Association and Dissociation of C ₆₀ Molecules S. Tsukamoto ¹ , M. Nakaya ^{1,2,3} , T. Nakayama ^{1,2,4} and M. Aono ^{1,2,3} , ¹ <i>NIMS</i> , ² <i>JST</i> , ³ <i>Osaka Univ.</i> and ⁴ <i>Univ. of Tsukuba, Japan</i> 380	380
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Session 6: Micro/nano-fabrications for device applications: ULSI fabrication processes, electronic, magnetic and optical devices (16:15 ~ 18:00)

Chair: S. Miyazaki (*Hiroshima Univ.*)

16:15	We-A20	Interface formations between $\text{Pr}_{0.7}\text{Ca}_{0.3}\text{MnO}_3$ epitaxial film and various metal electrodes toward resistance random access memory K. Tsubouchi ¹ , I. Ohkubo ¹ , H. Kumigashira ¹ , M. Oshima ¹ , K. Itaka ^{1,4} , Y. Matsumoto ^{2,4} , T. Ohnishi ¹ , M. Lippmaa ¹ and H. Koinuma ^{1,3,4} , ¹ <i>Univ. of Tokyo</i> , ² <i>Tokyo Inst. of Tech.</i> , ³ <i>NIMS</i> and ⁴ <i>CREST, JST, Japan</i> 383	383
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Chair: J. J. Ramsden (*Univ. Basel*)

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15:00	We-B15(I)	Structural and Functional Analysis of Genome Maintenance: A Single DNA Molecule Approach (Invited) A. Bensimon, <i>Genome Stability Unit, France</i> 392	392
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Chair: M. Niwano (*Tohoku Univ.*)

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Chair: A. Heinrich (*IBM*)

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- 9:30 Th-A2 Nanometer-Scale Control of Film Thickness and Pattern Width of Alkyl SAM on H-Terminated Si(111) Surface
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- 11:20 Th-A7(I) Mechanisms of Lateral Growth and Defect Generation in the Initial Oxidation of the Si(100) Surface (**Invited**)
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H. Kageshima¹, M. Uematsu¹, K. Akagi², S. Tsuneyuki², T. Akiyama³ and K. Shiraishi⁴,
¹*NTT Basic Research Labs,* ²*Univ. of Tokyo,* ³*Mie Univ. and* ⁴*Univ. of Tsukuba, Japan* 542
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Session 11: Surface chemistry and catalysis (9:00 ~ 12:20)

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V. Matolin^{1,2}, I. Matolinova^{1,2}, L. Sedlacek^{1,2}, N. Tsud¹ and T. Mori²,
¹*Charles Univ., Czech Republic and* ²*NIMS, Japan* 547

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Chair: M. Scheffler (*FHI*)

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Chair: H. Sakama (*Sophia Univ.*)

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9:45	Th-C4	Surface-state 1D plasmon on the Si(557)-Au surface T. Nagao ^{1,4} , S. Yaginuma ¹ , T. Inaoka ² , S. Hasegawa ³ and T. Sakurai ¹ , ¹ <i>Tohoku Univ.</i> , ² <i>Iwate Univ.</i> , ³ <i>Univ. of Tokyo and</i> ⁴ <i>ICORP, JST, Japan</i>	557
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11:35	Th-C9	Superlattice template epitaxy of strained GaSb dots on Si(001) K. Kawamoto ¹ , M. Jo ¹ , Y. Sugawara ^{1,2} and S. Fukatsu ^{1,2} , ¹ Univ. of Tokyo and ² PRESTO, JST, Japan.....	562
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Closing (12:20 ~ 13:00)

Chair: H. Onishi (*Kobe Univ.*)