PROGRAM

March 30, 2011 (Wed.)

14:00-18:00 **Registration**

18:00-20:00 **Welcome Reception**

March 31, 2011 (Thu.)

8:40-9:00 **Opening of the Conference**

Session I. Advanced TCAD Technology for Nano Devices I

Chair : Prof. Asen Asenov

09:00-09:30 I-01 Computational Electronics in the 21st Century: Status, Challenges and Opportunities

Mark Lundstrom

Network for Computational Nanotechnology and Birck Nanotechnology Center, Purdue University, West Lafayette, USA

09:30-10:00 I-02 Transient Simulation of the Electrical Double Layer: a New Path to Bio-sensing

Jun-Myoung Woo, Seok Hyang Kim, Jin Hong Ahn and Young June Park

Department of Electrical and Computer Engineering, Seoul National University, Korea

10:00-10:30 I-03 Density-Gradient Modeling and Complex Bandstructure Simulation of Tunneling Current in Device Simulation

Zhiping Yu

Institute of Microelectronics, Tsinghua University, Beijing, China

10:30-11:00 **Coffee Break**

Session II. Advanced TCAD Technology for Nano Devices II

Chair : Prof. Young June Park

11:00-11:30 I-04 Simulation of Statistical Variability and Reliability

Asen Asenov

Department of Electrical Engineering, University of Glasgow, Glasgow, UK

11:30-12:00 I-05 Development and Challenge on 3D Device and Process Simulation

Yasuyuki Okura

Semiconductor Leading Edge Technologies, Inc., Tsukuba, Japan

12:00-12:30 I-06 Advanced TCAD Modeling of Channel Mobility and External Resistance for 20nm-node CMOS Technology and Beyond

Seong-Dong Kim

Semiconductor R&D Center, IBM, NY, USA

12:30-14:00 **Lunch**

Session III. Advanced TCAD Technology for Nano Devices III

Chair : Prof. Mark Lundstrom

14:00-14:30 I-07 Advanced TCAD Simulation Beyond 1x nm Devices

Y. K. Park, H. S. Ahn, J. C. Kim, S. J. Kim, J. H. Kim, S. M. Kim and Y. W. Kwon

CAE Team, Semiconductor Division, Samsung Electronics, Korea

14:30-15:00 I-08 The Role of Technology CAD for Developing Present and Future Nano-Devices

Terry Ma, Victor Moroz, Ric Borges and Lee Smith

Synopsys, Inc., Mountain View, CA, USA

15:00-15:30 I-09 First Principle Studies on Interface Models for HfO_2 Gate Stack

Yongjin Park, Ki-jeong Kong, Hyunju Chang and Mincheol Shin[*]

Advanced Materials Division, Korea Research Institute of Chemical Technology, Daejeon, Korea

[*]*Department of Electrical Engineering, KAIST, Daejeon, Korea*

15:30-16:00 I-10 Nanodesign and Simulations toward Nanoelectronic Devices

Sang Uck Lee

Corporate R&D, LG Chem., Ltd., Research Park, Daejeon, Korea

16:00-16:30 **Coffee Break**

Session IV. Computational Research for Integrated Circuit Materials

Chair : Prof. Heiji Watanabe

16:30-17:00 I-11 Role of O-vacancy Defects in Devices Based on High-*k* Dielectrics and Amorphous Oxide Semiconductors

Kee Joo Chang, Byungki Ryu, Hyeon-Kyun Noh and Eun-Ae Choi[*]

Department of Physics, Korea Advanced Institute of Science and Technology, Daejeon, Korea

[*]*CAE Team, Memory Division, Samsung Electronics, Hwasung, Korea*

17:00-17:30 I-12 Computation of Capacitance at Nanometer Scale Using Orbital Partition Approach

Shusuke Kasamatsu[1], *Seungwu Han*[2], *and Satoshi Watanabe*[1]

[1]*Department of Materials Engineering, The University of Tokyo, Tokyo, Japan*

[2]*Department of Materials Science and Engineering, Seoul National University, Seoul, Korea*

Session V. Poster Session

Chair : Dr. Kwang-Ryeol Lee and Prof. Yuan Ping Feng

17:30-19:00 **Poster Session**

19:00-21:00 **Banquet (B.B.Q Restaurant 'B.B.Q. Garden')**

April 1, 2011 (Fri.)

Session VI. Transport Simulation for Nano and Molecular Devices I

Chair : Prof. Hiroshi Mizuseki

09:00-09:30 I-13 Quantum Transport of Holes in Nanoscale FETs: Dependence on Channel Orientation and Impact of Heavy-hole Light-hole Coupling

Mincheol Shin,

Department of Electrical Engineering, KAIST, Daejeon, Korea

09:30-10:00 I-14 Simulations on Time-varying Nanoscale Electronic Transport

S. Watanabe[1], W. Liu[1], D. Hirai[1], K. Sasaoka[1, 2] and T. Yamamoto[1]

[1]Department of Materials Engineering, the University of Tokyo, Tokyo, Japan

[2]Center for Computational Sciences, University of Tsukuba, Tsukuba, Japan

10:00-10:30 I-15 Self-energy Corrected Scattering-state Approach for Electrical and Thermal Transport Properties in Nanostructures

Hyoung Joon Choi

Department of Physics and IPAP, Yonsei University, Seoul, Korea

10:30-11:00 **Coffee Break**

Session VII. Transport Simulation for Nano and Molecular Devices II

Chair : Prof. Hyung Joon Choi

11:00-11:30 I-16 First-principles Study on Transport Properties of Nanoscale Conjugated Molecules

H. Mizuseki and Y. Kawazoe

Institute of Materials Research, Tohoku University, Sendai, Japan

11:30-12:00 I-17 Resolving Controversies on the Multiple Conductance Peaks in Single-Molecule Junction Experiments by Multiscale Simulations

Hu Sung Kim and Yong-Hoon Kim

Graduate School of EEWS, Korea Advanced Institute of Science and Technology, Daejeon, Korea

12:00-12:30 I-18 Transport Behavior in Kane-Mele Graphene Nanoribbons

Chen Hao

Physics Department, Fudan University, Shanghai, China

12:30-14:00 **Lunch**

Session VIII. Novel Materials for Next Generation Devices I

Chair : Prof. Vijay Kumar

14:00-14:30 I-19 How to Predict New Novel Materials for Next Generation Devices with Theoretical Confidence?

Y. Kawazoe

Institute of Materials Research, Tohoku University, Sendai, Japan

14:30-15:00 I-20 Anomalous Current Flow Patterns in Defected Carbon Nanotubes

Jisoon Ihm, Youngkuk Kim and Minsung Kim

Department of Physics and Astronomy, Seoul National University, Seoul, Korea

15:00-15:30 I-21 Simulation Design of Nanowires for Thermoelectric Device Applications

Gang Zhang

Key Laboratory for the Physics and Chemistry of Nanodevices and Department of Electronics, Peking University, Beijing, China

15:30-16:00 I-22 Atomic Structure and Band Gap Engineering in Graphene-BN Hybrid Nanostructures

Prashant P. Shinde and Vijay Kumar

Dr. Vijay Kumar Foundation, Haryana, India

16:00-16:30 **Coffee Break**

Session XI. Novel Materials for Next Generation Devices II

Chair : Prof. Young Woo Son

16:30-17:00 I-23 How to Functionalize Boron Nitride Sheet ant Nanotube for Device Applications

G. P. Das

Indian Association for the Cultivation of Science, Jadavpur, Kolkata, India

17:00-17:30 I-24 Graphene-Based Spin Logic Gates

Minggang Zeng[1,2], Lei Shen[1], Haibin Su[3,4], Miao Zhou[1], Chun Zhang[1,5] and Yuan Ping Feng[1]

[1]Department of Physics, National University of Singapore, Singapore

[2]NanoCore, National University of Singapore, Singapore

[3]Division of Materials Science, Nanyang Technological University, Singapore

[4]Institute of High Performance Computing, Singapore

[5]Department of Chemistry, National University of Singapore, Singapore

17:30-18:00 I-25 Graphitic Systems under External Perturbations: Energy Gaps and Electronic Topological Transition

Young-Woo Son

School of Computational Science, Korea Institute for Advanced Study, Seoul, Korea

April 2, 2011 (Sat.)

Session III Process Optimization by Computer Simulation I

Chair : Prof. Scott Dunham

09:00-09:30 I-26 Understanding and Control of Metal-Oxide-Semiconductor Interfaces for Advanced Nanoelectronics

Heiji Watanabe[1], Takuji Hosoi[1], Takayoshi Shimura[1], Kenji Shiraishi[2] and Keisaku Yamada[2]

[1]Graduate School of Engineering, Osaka University, Osaka, Japan

[2]Graduate School of Pure and Applied Sciences, University of Tsukuba, Tsukuba, Japan

09:30-10:00 I-27 Atomistic Stochastic Simulation of Front End Process

Alexander Schmidt, Hyo-Shin Ahn, Inkook Jang, Taikyung Kim and Young-Kwan Park

CAE Team, Semiconductor R&D Center, Samsung Electronics, Korea

10:00-10:30 I-28 Force Field Approaches for Modeling Oxide-Semiconductor Interfaces

Takanobu Watanabe[1,2]

[1]Faculty of Science and Engineering, Waseda University, Japan

[2]Institute of Nanoscience and Nanotechnology, Waseda University, Japan

10:30-11:00 **Coffee Break**

Session III Process Optimization by Computer Simulation II

Chair : Prof. Takanobu Watanabe

11:00-11:30 I-29 Atomistic Modeling of Nanodevice Fabrication

Scott T. Dunham and Renyu Chen

Department of Electrical Engineering, University of Washington, Seattle, USA

11:30-12:00 I-30 On Possibility for New Interface State of Si-dot Surrounded by Oxide

H. Watanabe

Department of Electrical Engineering, National Chiao Tung University, Taiwan

12:00-12:30 I-31 Reactive Molecular Dynamics Simulation of Oxide Formation on Silicon

Mauludi Ariesto, Byung-Hyun Kim, Gyubong Kim and Kwang-Ryeol Lee

Computational Science Center, Korea Institute of Science and Technology, Seoul, Korea

12:30-12:40 **Closing of Technical Sessions**

12:40-14:00 **Lunch**

14:00-17:00 **Guided Walking Tour of Jeju Olle-gil**

POSTER PRESENTATIONS

March 31, 2011 (Thu.)

P-01 Density functional theory determination of the electronic structure of zinc blende InN under high pressure

G. Zheng[1,2], J. Y. Guo[1,2], X. C. Wang[1,2]*

[1] School of Mathematics and Physics, China University of Geosciences, Wuhan 430074, China

[2] Institute of material modeling and computational physics, China University of Geosciences, Wuhan 430074, China

P-02 Molecular Dynamics Analysis of Nanotube-Based Nanoelectromechanical Memory Element

Jeong Won Kang[1], Jong Won Woon[2], Ho Jung Hwang[2]*

[1] Department of Computer Engineering, Chungju National University, Chungju 380-702, Korea

[2] School of Electrical and Electronic Engineering, Chung-Ang University, Korea

P-03 Electronic Band Structure of Si Nanosheets under External Strain

Mina Park[1], Gyubong Kim[1], Kwang-Ryeol Lee[1]*

[1] Computational Science Center, KIST, Korea

P-04 Effects of minimal perturbations on the energy-gap opening and the effective mass in graphene

Joon-Suh Park[1], Hyoung Joon Choi[1]*

[1] Department of Physics and IPAP, Yonsei University

P-05 Field-Induced Recovery of Massless Dirac Fermions in Epitaxial Graphene on SiC

Hyungjun Lee[1], Seungchul Kim[2], Jisoon Ihm[2], Young-Woo Son[3], Hyoung Joon Choi[1]*

[1] Department of Physics and IPAP, Yonsei University, Korea

[2] Department of Physics and Astronomy, Seoul National University, Korea

[3] Korea Institute for Advanced Study, Korea

P-06 Single-Impurity Scattering and Carrier Mobility in Doped Ge/Si Core-Shell Nanowires

Hyungjun Lee[*], Hyoung Joon Choi

Department of Physics and IPAP, Yonsei University, Korea

P-07 Atomistic simulations on static and dynamic properties of dislocations in bcc Fe

Jong Bae Jeon[*], Byeong Joo Lee, Young Won Chang

Department of Materials Science and Engineering, POSTECH, Korea

P-08 Local atomistic configuration effects on piezoelectric properties of $La_3Ta_{0.5}Ga_{5.5}O_{14}$ and a new piezoelectric crystal design

C.-Y. Chung[1], R. Yaokawa[2], H. Mizuseki[1], Y. Kawazoe[1]*

[1] Institute for materials research, Tohoku University, Japan

[2] Citizen Holdings Co. LTD., Japan

P-09 Spin Reorientation of Fe/MgO(001) System by the Formation of Oxygen Vacancy Row: an Ab Initio Study

Heechae Choi [*] and Yong-Chae Chung

Department of Materials Science and Engineering, Hanyang University, Seoul 133-791 Korea

P-10 Molecular dynamics simulation of the reconstruction of Si (111) surface by the constrained annealing treatment

Haining Cao[1,2], Kwang-Ryeol Lee[1], Byung-Hyun Kim[1], Mauludi Ariesto Pamungkas[1], M. Joe[1]*

[1] Computational Science Center, Korea Institute of Science and Technology, Republic of Korea

[2] International R&D Academy, University of Science and Technology, Daejeon 305-333, Republic of Korea

P-11 Reactive Molecular Dynamics Simulation of Early Stage of Dry Oxidation of Si (001) Surface

Mauludi Ariesto Pamungkas[1,2], Minwoong Joe[1], Byung-Hyun Kim[1], Gyubong Kim[1], and Kwang-Ryeol Lee[1,2]*

[1] Computational Science Center, Korea Institute of Science and Technology, Republic of Korea

[2] International R&D Academy, University of Science and Technology, Daejeon 305-333, Republic of Korea

P-12 Atomic-Scale Study of Nanocontact-induced Surface Defects in Iron and Copper

Chansun Shin[1], Hyung-ha Jin[1], Junhyun Kwon[1], Yuri Osetsky[2]*

[1] Nuclear Materials Division, Korea Atomic Energy Research Institute, Daejeon, Korea

[2] Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA

P-13 Molecular dynamics study of porous carbon growth for low-k materials

M. Joe[1], M.-W. Moon[1], and K.-R. Lee[1]*

[1] Computational Science Center, Korea Institute of Science and Technology, Seoul, Korea

P-14 Conduction in Disordered 3-D Topological Insulators

V. Sacksteder[1], S. Kettemann[2], X. Dai[3], Z. Fong[3], Q. Wu[3]*

[1] Institute of Physics, Chinese Academy of Sciences, Beijing 100190

[2] School of Engineering and Science, Jacobs University Bremen, Bremen 28759, Germany, and Division of Advanced Materials Science, Pohang University of Science and Technology (POSTECH), San31, Hyoja-dong, Nam-gu, Pohang 790-784, South Korea

[3] Beijing National Laboratory for Condensed Matter Physics, and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China

P-15 Theoretical DFT Study on Structure and Chemical Activity of Transition Metal Oxides, Carbon K4 and Metal-Organic Framework IRMOF Structures

Nurbosyn U. Zhanpeisov

Institute for International Education & Department of Chemistry,

Graduate School of Science, Tohoku University, Sendai 980-8576, Japan

P-16 First principle study on interaction between various metals and C atom in Me-Carbon System

Xiao-Wei Li[1, 2], Ai-Ying Wang[1], and Kwang-Ryeol Lee[2]*

[1] Ningbo Institute of Materials Technology and Engineering, CAS, Ningbo, P.R. China

[2] Computational Science Center, KIST, Seoul, Korea

P-17 Stability of donor-pair defects in $Si_{1-x}Ge_x$ alloy nanowires

Ji-Sang Park[1], Byungki Ryu[2], and Kee Joo Chang[1]*

[1] Department of Physics, Korea Advanced Institute of Science and Technology, Daejeon, Korea

[2] Samsung Advanced Institute of Technology, Suwon, Korea

P-18 Stability of boron dopants near the interface between Si and amorphous SiO_2

Y. J. Oh[*], H. K. Noh, and K. J. Chang

Department of Physics, Korea Advanced Institute of Science and Technology, Korea

P-19 First principle studies of $Si/SiO_2/HfO_2$ interface in MOSFET device

Yongjin Park[1], Ki-jeong Kong[1], Hyunju Chang[1], and Mincheol Shin[2]*

[1] Advanced Materials Div., Korea Research Institute of Chemical Technology, Korea

[2] Dept. of Electrical Engineering, KAIST, Korea

P-20 Understanding transient-enhanced boron diffusion in silicon by Molecular Dynamics simulations in Ultra-Shallow Junction (USJ) formation

Chansoo Kim[1], Byung-Joo Lee[2], Kwang-Ryeol Lee[1]*

[1] Computational Science Center, KIST, Korea

[2] Materials Science and Engineering, POSTECH, Korea

P-21 Molecular Dynamics Simulation Study of Silicon Nanowires Oxidation

Byung-Hyun Kim[1,2], Gyubong Kim[1], Mina Park[1], Mauludi Ariesto Pamungkas[1,3], Kwang-Ryeol Lee[1], and Yong-Chae Chung[2]*

[1] Computational Science Center, Interdisciplinary Fusion Technology Division, KIST, Korea

[2] Department of Materials Science and Engineering, Hanyang University, Korea

[3] Department of Nanomaterial Science and Technology, University of Science and Technology, Korea

P-22 Atomic Scale Investigation of the Si/SiO_x Interface in Silicon Nanowire

Byung-Hyun Kim[1,2], Gyubong Kim[1], Mina Park[1], Mauludi Ariesto Pamungkas[1,3], Kwang-Ryeol Lee[1], and Yong-Chae Chung[2]*

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P-23 Introduction to the Joint Research Project for the Development of Molecular Simulation Technology for Nano Devices

Kwang-Ryeol Lee[1], Hyunju Chang[2], Mincheol Shin[3] and Kee Joo Chang[4]

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