Mini-symposium B3
Multiscale Simulation for Nano-device Design

Organizers:
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Fri - 9 Jan 2015 | 11:00 – 12:30 | Room 04-30/32/34, Block S16

Chair: Satoshi Watanabe

11:00 B3-01 Keynote
Multiscale simulation of statistical reliability in nanoscale transistors: From atoms to circuit reliability
Asen Asenov  
Gold Standard Simulations Ltd, James Watt Professor, The University of Glasgow

11:30 B3-02 Invited
Multiscale study of doped carbon nanomaterials for novel device applications
Yong-Hoon Kim  
Graduate School of EEWS, KAIST, 291 Daehak-ro, Yuseong-gu, Daejeon 305-701, Korea

12:00 B3-03
Simulation Platform of Nano-devices as the Virtual Fab
Minho Lee, Seungchul Lee, Mincheol Shin, Kwang-Ryeol Lee  
Center for Computational Science, Institute of Multidisciplinary Convergence of Matter, Korea Institute of Science and Technology, 39-1 Hawolgok-dong, Seongbuk-gu, Seoul, Korea

Fri - 9 Jan 2015 | 14:00 – 15:30 | Room 04-30/32/34, Block S16

Chair: Asen Asenov

14:00 B3-05 Invited
Scattering Basis Representation in Quantum Transport Simulation of Nanowire Transistors
Nobuya Mori1,2, Gennady Mil'nikov1,2  
1Osaka University, 2CREST, JST

14:30 B3-06 Invited
Multiscale simulation of Schottky barrier tunnel transistors
Mincheol Shin1, Pooja Srivastava2, Junbeom Seo1, Jaechyun Lee1, Seungchul Kim2, Kwang-Ryeol Lee2  
1Korea Advanced Institute of Science and Technology 291 Daehak-ro, Yuseong, Daejeon 305-701, Rep. of Korea; 2Korea Institute of Science and Technology 14-gil 5 Hwarang-ro, Seongbuk, Seoul 136-79, Rep. of Korea

15:00 B3-07
Simulation of nanopore transistors: ion current modulation by the embedded gate electrode
Yong Youn, Dongsun Yoo, Seungwu Han†  
Department of Materials Science and Engineering, Seoul National University, Seoul 151-744, Korea

15:15 B3-08
Simulation and design of THz emitters based on the GaN HEMT structure
Sung-Min Hong, Jae-Hyung Jang  
School of Information and Communications, Gwangju Institute of Science and Technology, 123 Cheomdan-gwagiro(Oryong-dong), Buk-gu, Gwangju 500-712, Korea
11:00 B3-09 Keynote

**Density Functional Study on Tantalum Oxide based Resistive Switching Devices**

Satoshi Watanabe, Bo Xiao  
*Department of Materials Engineering, The University of Tokyo / 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan*

11:30 B3-10 Invited

**Density Functional Theory for the Steady State of Quantum System under a Finite Bias**

Chun Zhang  
*Department of Physics, National University of Singapore, and Department of Chemistry, National University of Singapore*

12:00 B3-11

**Atomistic Modeling of Silicon Grain Boundaries for Solar Cell Devices**

Hiroshi Mizuseki¹, Yoshiyuki Kawazoe²  
¹Center for Computational Science, Korea Institute of Science and Technology (KIST), Hwarangno 14-gil 5, Seongbuk-gu, Seoul, 136-791, Republic of Korea, ²New Industry Creation Hatchery Center, Tohoku University, 6-6-4 Aoba, Aramaki, Aoba-ku, Sendai, 980-8579, Japan

12:15 B3-12

**Computational study of the surface morphology of graphene on amorphous silica**

Ji Il Choi¹, Yoonsu Shim¹, Young-Jun Yu², Seok Hoon Ahn³, Yong-Hoon Kim¹  
¹Graduate School of EEWS, KAIST, Daejeon, Korea, ²Creative Research Center for Graphene Electronics, ETRI, Daejeon, Korea, ³Soft Innovative Materials Research Center, KIST, Jeonbuk, Korea

14:00 B3-13 Invited

**Multiscale modeling in computational biology and drug design**

Art E. Cho  
*Korea University / 2511 Sejong-ro, Sejong, 339-700 Korea*

14:30 B3-14

**Designing the nanodevices by understanding the charge redistribution between self-assembling adsorbates and supporting substrates**

Jia-Tao Sun  
*Institute of Physics, Chinese Academy of Sciences, Beijing, China*

14:45 B3-15

**Electron Transport Characteristics of Nano-flake embedded Graphene Nanoribbons**

Sang Uck Lee  
*Department of Applied Chemistry, Hanyang University, 55 Hanyangdaehak-ro, Sangnok-gu, Ansan 426-791 Korea*

15:00 B3-16

**Modeling the Performance of Highly Stretchable and Sensitive Sensors Based on Metal Nanowire-Elastomer Nanocomposite**

Sangryun Lee, Morteza Amjadi, Inkyu Park, Seunghwa Ryu  
*Mechanical Engineering, KAIST, Daejeon, Korea*