SYMPOSIUM AGENDA

International Symposium on Computics: Quantum Simulation and Design (ISC-QSD)

Thursday, 11 October 2012

1100-1250		*Registration for Symposium at the registration desk*

Opening session

1250-1320		Opening address, and Material design through computics Atsushi Oshiyama (Univ. of Tokyo, Tokyo, Japan)

Session I (Computer architecture and numerical algorithm)

[Chair: M. Inaba]

1320-1350	I-1	George Chiu (IBM, Yorktown Heights, USA) *IBM Blue Gene/Q Platform*
1350-1420	I-2	Takeo Hoshi (Tottori Univ., Tottori, Japan) *Ten-million-atom electronic structure calculations with novel linear-algebraic algorithm and the K computer*
1420-1440	O-1	Yasuo Ishii (Univ. of Tokyo, Tokyo, Japan) *High Performance, Energy-Efficient and Scalable Memory Subsystem Design for Many-Core Processors*
1440-1500	O-2	Tomohiro Sogabe (Aichi Prefectural Univ., Aichi, Japan) *Krylov subspace methods for generalized shifted linear systems arising in large-scale electronic structure calculation*
1500-1530		*Coffee Break*

Session II (Large scale calculation)

[Chair: T. Ono]

1530-1600	I-3	Stefan Bluegel (PGI-1 and IAS-1, Juelich, Germany) *KKRnano: Precise massively parallel density functional calculations for thousands of atoms*
1600-1630	I-4	Mike Gillan (UCL, London, UK) *Linear-scaling DFT on systems of over a million atoms with the CONQUEST code*

1630-1650 O-3 Tsuyoshi Miyazaki (NIMS, Tsukuba, Japan)
Recent Developments in a linear scaling DFT code CONQUEST

[Chair: Y. Yoshimoto]

1650-1720 I-5 Junichi Iwata, (Univ. of Tokyo, Tokyo, Japan)
Band structure calculations of large-scale systems by Sakurai-Sugiura method

1720-1750 I-6 Markus Eisenbach (Oak Ridge National Lab., Tennessee, USA)
Future Proofing WL-LSMS: Preparing for First Principles Thermodynamics Calculations on Accelerator and Multicore Architectures

Friday, 12 October 2012

0830-0900 *Registration for Symposium at the registration desk*

Session III (Transport properties)

[Chair: S. Watanabe]

0900-0930 I-7 GuanHua Chen (Univ. of Hong Kong, Hong Kong, China)
QM/EM method and its application

0930-0950 O-4 Tomoya Ono (Osaka Univ., Osaka, Japan)
First-principles transport calculation method using real-space finite-difference NEGF scheme

0950-1010 O-5 Kenji Sasaoka (Univ. of Tokyo, Tokyo, Japan)
Non-Equilibrium Green's Function Simulations of Non-Linear AC Current through a Quantum Dot

1010-1030 *Coffee Break*

Session IV (Materials Design)

[Chair: K. Sato]

1030-1100 I-8 Lin-Wang Wang (LBNL, Berkeley, USA)
Large scale electronic structure calculations for nanosystems

1100-1130 I-9 Xin-Gao Gong (Fudan Univ., Shanghai, China)
Theoretical Understanding of Multinary Alloys for the Solar Absorbers

1130-1150 O-6 Kazuyuki Uchida (Univ. of Tokyo, Tokyo, Japan)
Atom-scale identification of In/Si(111)-r7xr3 surface

1150-1210 O-7 Yoshihiro Gohda (Univ. of Tokyo, Tokyo, Japan)
New phase of graphene at interfaces with GaN

1210-1230 O-8 Tatsuki Oda (Kanazawa Univ., Kanazawa, Japan)
Electric-field effects on magnetic anisotropy in FePd and FePt ultrathin films

1230-1240 ***Official Photo taking at the entrance of the Osaka University Hall***

1240-1400 *Lunch*

1400-1600 **Poster Session at the assembly hall**
(Coffee will be served)

Session V (Dynamics)

[Chair: S. Tsuneyuki]

1600-1630 I-10 Fabio Pietrucci (CECAM-EPFL, Lausanne, Switzerland)
Combining graph theory with ab initio molecular dynamics: discovery of a new route for the transformation of graphene into fullerene

1630-1700 I-11 Kazuhiro Yabana (Univ. of Tsukuba, Tsukuba, Japan)
Multi-scale first-principles approach for strong electromagnetic field in solids

1700-1720 O-9 Hiroshi Nakanishi (Osaka Univ., Osaka, Japan)
Quantum simulation for proton and muon on solid surfaces and in subsurfaces

Session VI (Biological system)

[Chair: T. Yamato]

1720-1750 I-12 H. C. Watanabe
(Karlsruhe Institute of Technology, Karlsruhe, Germany)
Computational challenge of protein structural modeling

1800-2000 *Symposium banquet at the assembly hall in the Osaka University Hall*

Saturday, 13 October, 2012

0830-0900		*Registration for Symposium at the registration desk*

Session VII (New development in DFT and strongly correlated system)

[Chair: M. Imada]

0900-0930	I-13	Silke Biermann (CPHT, Paris, France)
0930-1000	I-14	Arno Schindlmayr (Univ. Paderborn, Paderborn, Germany) *Efficient first-principles calculation of electronic excitation within the all-electron FLAPW method*
1000-1030	I-15	Thomas Pruschke (Univ. of Göttingen, Germany) *Density-matrix functional theory as novel approach to combine first-principle methods with correlations*
1030-1050		Coffee *Break*

[Chair: Y. Takada]

1050-1110	O-10	Naoto Tsuji (Univ. of Fribourg, Fribourg, Switzerland) *Dynamical phase transition and nonthermal steady states in the Hubbard model*
1110-1140	I-16	Michele Casula (CNRS, Paris, France) *Electron-phonon coupling in potassium-doped superconducting picene*
1140-1200	O-11	Kazuma Nakamura (Univ. of Tokyo, Tokyo, Japan) *Ab initio low-energy models for organic materials*
1200-1220	O-12	Ryo Maezono (JAIST, Ishikawa, Japan) *Non-additivity in metallic tri-wire binding*

Closing session

1220-1230		Summary
		Symposium Closes