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<th>June 14 (Tuesday)</th>
<th>Oral Session (including Opening Ceremony)</th>
<th>Welcome Party</th>
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<tr>
<td>June 15 (Wednesday)</td>
<td>Oral Session</td>
<td>Poster Session</td>
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<td>June 16 (Thursday)</td>
<td>Oral Session</td>
<td>Poster Session</td>
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<td>June 17 (Friday)</td>
<td>Oral Session</td>
<td>Banquet</td>
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<td>June 18 (Saturday)</td>
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### Oral Session (including Opening Ceremony)

**Date:** June 14 (Tuesday) 16:10 - 18:20  
**Location:** Noh Theatre

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<th>Time</th>
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<tr>
<td>16:10</td>
<td>Opening Remarks</td>
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<tr>
<td>16:10 - 16:20</td>
<td>Fumio HIRATA (IMS &amp; GUAS, Okazaki)</td>
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<td>16:20</td>
<td>Greeting</td>
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<td>16:20 - 16:30</td>
<td>Kaneyuki MATSUWA (MEXT, Japan)</td>
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<td>16:30</td>
<td>Greeting</td>
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<tr>
<td>16:30 - 16:40</td>
<td>Hiroki NAKAMURA (IMS &amp; GUAS, Okazaki)</td>
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<td>16:40</td>
<td>National Research Grid Initiative (NAREGI) (PL03)</td>
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<td>16:40 - 17:30</td>
<td>Kenichi MIURA (NII, Tokyo (Project Leader, NAREGI))</td>
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<tr>
<td>17:30</td>
<td>Towards Science Based Intellectual Manufacturing - Expectations on NAREGI and High End Computing - (PL04)</td>
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<tr>
<td>17:30 - 18:20</td>
<td>Michiharu NAKAMURA (Hitachi, Ltd.)</td>
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<td>18:20</td>
<td>Welcome Party (Reception Hall)</td>
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<tr>
<td>18:20 - 20:00</td>
<td>Greeting &amp; Toast, Koji KAYA (RIKEN, Wako)</td>
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**TOP**
June 15 (Wednesday) 09:00 - 18:00  Oral Session

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<tr>
<th>Time</th>
<th>Noh Theatre</th>
<th>Room A</th>
<th>Room B</th>
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<tbody>
<tr>
<td>09:00 - 09:50</td>
<td><strong>Computational Nanoscience, NAREGI (PL01)</strong>&lt;br&gt;<strong>Chair: Masaru NAKAHARA (Kyoto Univ.)</strong>&lt;br&gt;<strong>Fumio HIRATA</strong> (IMS &amp; GUAS, Okazaki (Principal Investigator, NAREGI))</td>
<td><strong>Condensed Matter Theory</strong>&lt;br&gt;<strong>Chair: Yoshiyuki MIYAMOTO (NEC Corp.)</strong>&lt;br&gt;<strong>Theory and Computation of the Optical, Transport, and Mechanical Properties of Nanostructures (IL-CMT06)</strong></td>
<td><strong>Quantum Chemistry</strong>&lt;br&gt;<strong>Chair: Shigeru NAGASE (IMS &amp; GUAS, Okazaki)</strong>&lt;br&gt;DFT, DFTB and ONIOM Studies of Nanostructures (tentative) (IL-QC08)</td>
<td><strong>Molecular Dynamics Simulations, Statistical Mechanics of Solutions, Experiments</strong>&lt;br&gt;<strong>Chair: Haruki NAKAMURA (Osaka Univ.)</strong>&lt;br&gt;Atomistic Nanoscale Simulations of Lipid Bilayers (IL-MSE02)</td>
</tr>
<tr>
<td>09:50 - 10:40</td>
<td><strong>The World of Soft Nano-Material (PL02)</strong>&lt;br&gt;<strong>Koji KAYA</strong> (RIKEN)</td>
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<td>10:40 - 11:00</td>
<td><strong>Coffee Break</strong></td>
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<tr>
<td>11:00 - 11:40</td>
<td><strong>Condensed Matter Theory</strong>&lt;br&gt;<strong>Chair: Yoshiyuki MIYAMOTO (NEC Corp.)</strong>&lt;br&gt;<strong>Theory and Computation of the Optical, Transport, and Mechanical Properties of Nanostructures (IL-CMT06)</strong></td>
<td><strong>DFT, DFTB and ONIOM Studies of Nanostructures (tentative) (IL-QC08)</strong>&lt;br&gt;<strong>Keiji MOROKUMA</strong> (Emory Univ., Atlanta)</td>
<td><strong>Molecular Dynamics Simulations, Statistical Mechanics of Solutions, Experiments</strong>&lt;br&gt;<strong>Chair: Haruki NAKAMURA (Osaka Univ.)</strong>&lt;br&gt;<strong>Olle EDHOLM</strong> (KTH-SCFAB, Stockholm)</td>
<td><strong>Atomistic Nanoscale Simulations of Lipid Bilayers (IL-MSE02)</strong>&lt;br&gt;<strong>James R. CHELIKOWSKY</strong> (Univ. of Texas at Austin)</td>
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<tr>
<td>11:40 - 12:20</td>
<td><strong>Magnetically Doped Quantum Dots (IL-CMT04)</strong>&lt;br&gt;<strong>James R. CHELIKOWSKY</strong> (Univ. of Texas at Austin)</td>
<td><strong>Theoretical Inspect into Catalysis of Transition Metal Complexes (IL-QC11)</strong>&lt;br&gt;<strong>Shigeyoshi SAKAKI</strong> (Kyoto Univ.)</td>
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<td>12:20 - 14:00</td>
<td><strong>Lunch</strong></td>
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<td>14:00 - 14:40</td>
<td>Noh Theatre</td>
<td>Functional Nanomolecule (KL03)</td>
<td>Yuko OKAMOTO (Nagoya Univ.)</td>
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<td>14:40 - 15:20</td>
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<td>Molecular Dynamics and Statistical Mechanical Studies on Structure and Dynamics of Nano-Scale Molecular Assemblies in Solution by NAREGI Nanoscience Project (KL04)</td>
<td>Susumu OKAZAKI (IMS &amp; GUAS, Okazaki)</td>
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<td>15:20 - 15:40</td>
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<tr>
<td>15:40 - 16:20</td>
<td>Room A</td>
<td>Modeling of Complex Microstructure Changes in Metallic Materials Using the Phase-Field Method (IL-CMT05)</td>
<td>Katsuyuki NOBUSADA (IMS &amp; GUAS, Okazaki)</td>
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<td>16:20 - 17:00</td>
<td>Room B</td>
<td>Hybrid Quantum-Classical Simulation over the Pacific Grid (IL-CMT09)</td>
<td>Toshiyuki KOYAMA (Nat. Inst. for Materials Sci., Tsukuba)</td>
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<td>17:00 - 17:20</td>
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<td>Coffee Break</td>
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<td>17:20 - 18:00</td>
<td>Room C</td>
<td>Dynamical Properties of the Electron Liquid: Importance of the Excitonic Effect (IL-CMT12)</td>
<td>Keiichiro NASU (Inst. of Materials Structure Sci., KEK, Tsukuba)</td>
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<td>18:00 - 18:20</td>
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<td>18:20 - 20:00</td>
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<td>Poster Session 1 (Reception Hall, Snack and Drink Served)</td>
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### June 16 (Thursday) 10:10 - 17:30  Oral Session

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<th>Time</th>
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<tbody>
<tr>
<td>10:10</td>
<td>Chair: Shi-aki HYODO (TOYOTA Cent. R&amp;D Labs)</td>
<td>Chair: Keiji MOROKUMA (Emory Univ., Atlanta)</td>
<td>Chair: Shinichi MIURA (IMS &amp; GUAS, Okazaki)</td>
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<td>Forces and Structure in Nematic-Colloid Dispersions (IL-MSE14)</td>
<td>The Chemistry of Carbodiphosphoranes: Theoretical Studies of Unexplored Territory (IL-QC03)</td>
<td>Computer Simulation Studies of the Self-Assembly of Natural and Synthetic Membranes (IL-MSE06)</td>
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<tr>
<td>10:10 - 10:50</td>
<td>Grenfel N. PATEY (Univ. of British Columbia, Canada)</td>
<td>Gernot FRENKING (Fachbereich Chem. Philipps-Univ. Marburg)</td>
<td>Michael L. KLEIN (Univ. of Pennsylvania)</td>
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<td>Water Dynamics; Potential Energy Landscape and Fluctuation (IL-MSE12)</td>
<td>Recent Advances in Electronic Structure Theory (IL-QC05)</td>
<td>Pase Behaviors of Confined Water (IL-MSE18)</td>
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<td>Iwao OHMINE (Nagoya Univ.)</td>
<td>Kimihiko HIRAO (Univ. of Tokyo)</td>
<td>Hideki TANAKA (Okayama Univ.)</td>
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<td>11:30 - 13:30</td>
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<td>13:30</td>
<td>Chair: Kenji YONEMITSU (IMS &amp; GUAS, Okazaki)</td>
<td>Grid Computing Management (KL02)</td>
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<td>13:30 - 14:10</td>
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<td>Fumiyasu MIZUTANI (IMS, Okazaki)</td>
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<td>Nano-Magnetism (KL05)</td>
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<td>14:10 - 14:50</td>
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<td>Hajime TAKAYAMA (Univ. of Tokyo)</td>
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<td>Chair: Takami TOHYAMA (Tohoku Univ.)</td>
<td>Chair: Nobuyuki MATUBAYASI (Kyoto Univ.)</td>
<td>Chair: Hideki TANAKA (Okayama Univ.)</td>
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<td>Quantum Monte Carlo for Strongly Correlated Electrons (tentative) (IL-CMT11)</td>
<td>Quantum Simulation of Molecular Clusters (IL-MSE16)</td>
<td>Large-scale MD Simulation of Mass and Heat Transfer at Interfaces (IL-MSE08)</td>
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<td>Sandro SORELLA (SISSA, Trieste)</td>
<td>Peter J. ROSSKY (Univ. of Texas at Austin)</td>
<td>Mitsuhiro MATSUMOTO (Kyoto Univ.)</td>
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<td>Time</td>
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<td>Path Integral Hybrid Monte Carlo Study of Solvated Molecules in Superfluid Helium-4 Clusters (IL-MSE10)</td>
<td>Shinichi MIURA (IMS &amp; GUAS, Okazaki)</td>
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<td>Computational Approaches to Vibrational Spectroscopy in Water: Line Shapes and Echoes (IL-MSE17)</td>
<td>James L. SKINNER (Univ. of Wisconsin)</td>
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<tr>
<td>16:30 - 16:50</td>
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<td>16:50 - 17:30</td>
<td>Finite-Temperature Dynamics in Microscopic Model for Cuprates: Small-System Results (IL-CMT10)</td>
<td>Peter PRELOVSEK (Jozef Stefan Inst., Ljubljana)</td>
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<td>DFT Calculations of the Electronic Properties of SWNTs: Beyond the Local Density Approximation (IL-QC13)</td>
<td>Gustavo E. SCUSERIA (Rice Univ., Houston)</td>
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<td>Free-Energy Calculation in Solution with the Method of Energy Representation (IL-MSE09)</td>
<td>Nobuyuki MATUBAYASI (Kyoto Univ.)</td>
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<td>Coffee Break</td>
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<td>17:50 - 19:30</td>
<td>Poster Session 2 (Reception Hall, Snack and Drink Served)</td>
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June 17 (Friday) 09:00 - 17:30  Oral Session

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<th>Time</th>
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<tr>
<td>09:00</td>
<td>Chair: Sadamichi MAEKAWA (Tohoku Univ.)</td>
<td>Chair: Mutsumi AOYAGI (Kyushu Univ.)</td>
<td>Chair: Fumio HIRATA (IMS &amp; GUAS, Okazaki)</td>
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<tr>
<td>09:00</td>
<td>Pushing Back the Frontiers of Molecular Dynamics Simulation (PL05)</td>
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<td>09:00</td>
<td>Michele PARRINELLO (Eidgenössische Tech. Hochschule Zürich)</td>
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<td>13:30</td>
<td>Chair: Hajime TAKAYAMA (Univ. of Tokyo)</td>
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<td>13:30</td>
<td>Nano-System Designing (KL06)</td>
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<td>Kiyoyuki TERAKURA (AIST, Tsukuba)</td>
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<td>14:10</td>
<td>Sadamichi MAEKAWA (Tohoku Univ.)</td>
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<td>15:10</td>
<td>Chair: Hisazumi AKAI (Osaka Univ.)</td>
<td>Chair: Shigeki KATO (Kyoto Univ.)</td>
<td>Chair: Akihiro MORITA (IMS &amp; GUAS, Okazaki)</td>
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<tr>
<td>15:10 - 15:50</td>
<td><strong>Mesoscopic Physics with Rare-Earths</strong> (IL-CMT01)</td>
<td><strong>Fullerenes and Nanotubes, Arena not only for Experimentalists but also for Theoreticians</strong> (IL-QC02)</td>
<td><strong>Hydrophobic Association of Mesoscopic Solutes</strong> (IL-MSE15)</td>
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<td><strong>Bernard BARBARA</strong> (Lab. Louis Neel-CNRS, Grenoble)</td>
<td><strong>Zhongfang CHEN</strong> (Univ. of Georgia)</td>
<td><strong>B. Montgomery PETTITT</strong> (Univ. of Houston)</td>
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<td>15:50</td>
<td><strong>Quantum Relaxation and Schrödinger's Cat States of Single-Molecule Magnets</strong> (IL-CMT07)</td>
<td><strong>Grid Enabling of RISM-FMO Coupled Simulation</strong> (IL-QC01)</td>
<td><strong>Computing Grid towards Multi-Level / Multi-Scale Biological Simulations</strong> (IL-MSE11)</td>
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<td><strong>Fernando LUIS</strong> (CSIC-Univ. de Zaragoza)</td>
<td><strong>Mutsumi AYOAGI</strong> (Kyushu Univ.)</td>
<td><strong>Haruki NAKAMURA</strong> (Osaka Univ.)</td>
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<td>16:00</td>
<td><strong>Coffee Break</strong></td>
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<td>16:00 - 16:50</td>
<td>Chair: Seiji MIYASHITA (Univ. of Tokyo)</td>
<td>Chair: Hiromi NAKAI (Waseda Univ.)</td>
<td>Chair: Akihiro MORITA (IMS &amp; GUAS, Okazaki)</td>
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<td>16:50</td>
<td><strong>Photogeneration of Ferroelectric and Conductive Nano Domain in SrTiO₃</strong> (IL-CMT08)</td>
<td><strong>Potential Energy Surfaces and Electronic Relaxation Dynamics of Transition Metal Ion Aqueous Solution</strong> (IL-QC06)</td>
<td><strong>Statistical Mechanical Theory of Solutions: a Key to Multiple-Scale Modeling of Thermo- and Electrochemistry in Disordered Nanoporous Materials</strong> (IL-MSE07)</td>
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<td><strong>Qui YU and Keiichiro NASU</strong> (Inst. of Materials Structure Sci., KEK, Tsukuba)</td>
<td><strong>Shigeki KATO</strong> (Kyoto Univ.)</td>
<td><strong>Andriy KOVALENKO</strong> (NINT, Nat. Res. Council Canada)</td>
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<td><strong>Coffee Break</strong></td>
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<td>17:30 - 17:50</td>
<td><strong>Banquet (Reception Hall)</strong></td>
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| 09:00 - 17:30 | KOYASAN (Mount KOYA), Historic Shingon Temples (UNESCO World Heritage):  
              | See, for example, URL: http://www.shukubo.jp/eng/index.html.  
              | Details will be appeared soon.                                                               |
### TOPIC AREA

**Quantum Chemistry (QC)**

- Molecular Dynamics Simulations (MD)
- Statistical Mechanics of Solutions (SMS)
- Condensed Matter Theory (CMT)

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<td><strong>Molecular Dynamics Simulations (MD)</strong></td>
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<td><strong>Statistical Mechanics of Solutions (SMS)</strong></td>
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<td><strong>Condensed Matter Theory (CMT)</strong></td>
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June 16 (Thursday)

17:50 - 19:30 Poster Session 2

**TOPIC AREA**
- **Quantum Chemistry (QC)**
- **Molecular Dynamics Simulations (MD)**
- **Statistical Mechanics of Solutions (SMS)**
- **Condensed Matter Theory (CMT)**

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<td>Condensed Matter Theory (CMT)</td>
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### List of Plenary Speakers

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<thead>
<tr>
<th>PL01</th>
<th>Fumio HIRATA</th>
<th>IMS &amp; GUAS, Okazaki (Principal Investigator, NAREGI)</th>
<th>Computational Nanoscience, NAREGI</th>
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<tbody>
<tr>
<td>PL02</td>
<td>Koji KAYA</td>
<td>RIKEN, Wako</td>
<td>The World of Soft Nano-Material</td>
</tr>
<tr>
<td>PL03</td>
<td>Kenichi MIURA</td>
<td>NII, Tokyo (Project Leader, NAREGI)</td>
<td>National Research Grid Initiative (NAREGI)</td>
</tr>
<tr>
<td>PL04</td>
<td>Michiharu NAKAMURA</td>
<td>Hitachi Ltd.</td>
<td>Towards Science Based Intellectual Manufacturing - Expectations on NAREGI and High End Computing -</td>
</tr>
<tr>
<td>PL05</td>
<td>Michele PARRINELLO</td>
<td>Eidgenössische Tech. Hochschule Zürich</td>
<td>Pushing Back the Frontiers of Molecular Dynamics Simulation</td>
</tr>
</tbody>
</table>

### List of Invited Speakers (Quantum Chemistry (QC))

<table>
<thead>
<tr>
<th>IL-QC01</th>
<th>Mutsumi AOYAGI</th>
<th>Kyushu Univ.</th>
<th>Grid Enabling of RISM-FMO Coupled Simulation</th>
</tr>
</thead>
<tbody>
<tr>
<td>IL-QC02</td>
<td>Zhongfang CHEN</td>
<td>Univ. of Georgia</td>
<td>Fullerenes and Nanotubes, Arena not only for Experimentalists but also for Theoreticians</td>
</tr>
<tr>
<td>IL-QC03</td>
<td>Gernot FRENKING</td>
<td>Fachbereich Chem. Philipps-Univ. Marburg</td>
<td>The Chemistry of Carbodiphosphoranes: Theoretical Studies of Unexplored Territory</td>
</tr>
<tr>
<td>IL-QC04</td>
<td>Mark S. GORDON</td>
<td>Ames Lab. &amp; Iowa State Univ.</td>
<td>Scalable Correlated Electronic Structure Theory: Strategies and Applications</td>
</tr>
<tr>
<td>IL-QC05</td>
<td>Kimihiko HIRAO</td>
<td>Univ. of Tokyo</td>
<td>Recent Advances in Electronic Structure Theory</td>
</tr>
<tr>
<td>IL-QC06</td>
<td>Shigeki KATO</td>
<td>Kyoto Univ.</td>
<td>Potential Energy Surfaces and Electronic Relaxation Dynamics of Transition Metal Ion Aqueous Solution</td>
</tr>
<tr>
<td>IL-QC07</td>
<td>Kazuo KITAURA</td>
<td>AIST, Tsukuba</td>
<td>Fragment MO Method and its Application to Proteins</td>
</tr>
<tr>
<td>IL-QC08</td>
<td>Keiji MOROKUMA</td>
<td>Emory Univ., Atlanta</td>
<td>DFT, DFTB and ONIOM Studies of Nanostructures (tentative)</td>
</tr>
<tr>
<td>IL-QC09</td>
<td>Hiromi NAKAI</td>
<td>Waseda Univ.</td>
<td>Development of Accurate Non-Born-Oppenheimer Theory and Its Applications</td>
</tr>
<tr>
<td>IL-QC10</td>
<td>Peter PULAY</td>
<td>Univ. of Arkansas</td>
<td>Calculation of the Dispersion Interaction in Large Molecules</td>
</tr>
<tr>
<td>IL-QC11</td>
<td>Shigeyoshi SAKAKI</td>
<td>Kyoto Univ.</td>
<td>Theoretical Inspect into Catalysis of Transition Metal Complexes</td>
</tr>
<tr>
<td>Code</td>
<td>Name</td>
<td>Institution</td>
<td>Title</td>
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<tr>
<td>IL-QC12</td>
<td>Paul V. R. SCHLEYER</td>
<td>Univ. of Georgia</td>
<td>The Aromaticity and Anti-Aromaticity of Clusters</td>
</tr>
<tr>
<td>IL-QC13</td>
<td>Gustavo E. SCUSERIA</td>
<td>Rice Univ., Houston</td>
<td>DFT Calculations of the Electronic Properties of SWNTs: Beyond the Local Density Approximation</td>
</tr>
</tbody>
</table>

**List of Invited Speakers**

(Molecular Dynamics Simulations, Statistical Mechanics of Solutions, Experiment (MSE))

<table>
<thead>
<tr>
<th>Code</th>
<th>Name</th>
<th>Institution</th>
<th>Title</th>
</tr>
</thead>
<tbody>
<tr>
<td>IL-MSE01</td>
<td>Peter T. CUMMINGS</td>
<td>Vanderbilt Univ. &amp; Oak Ridge Nat. Lab.</td>
<td>Computational and Theoretical Nanoscience: Methods and Applications</td>
</tr>
<tr>
<td>IL-MSE02</td>
<td>Olle EDHOLM</td>
<td>KTH-SCFAB, Stockholm</td>
<td>Atomistic Nanoscale Simulations of Lipid Bilayers</td>
</tr>
<tr>
<td>IL-MSE03</td>
<td>James T. HYNES</td>
<td>ENS, Paris &amp; Univ. of Colorado at Boulder</td>
<td>Solvation and Photochemical Funnels: Environmental Effects on Conical Intersection Structure and Dynamics</td>
</tr>
<tr>
<td>IL-MSE04</td>
<td>Shi-aki HYODO</td>
<td>TOYOTA Cent. R&amp;D Labs</td>
<td>Hierarchical Structural Simulation for Materials</td>
</tr>
<tr>
<td>IL-MSE05</td>
<td>Masahiro KINOSHITA</td>
<td>Kyoto Univ.</td>
<td>A Powerful Driving Force in Protein Folding</td>
</tr>
<tr>
<td>IL-MSE06</td>
<td>Michael L. KLEIN</td>
<td>Univ. of Pennsylvania</td>
<td>Computer Simulation Studies of the Self-Assembly of Natural and Synthetic Membranes</td>
</tr>
<tr>
<td>IL-MSE07</td>
<td>Andriy KOVALENKO</td>
<td>NINT, Nat. Res. Council Canada</td>
<td>Statistical Mechanical Theory of Solutions: a Key to Multiple-Scale Modeling of Thermo- and Electrochemistry in Disordered Nanoporous Materials</td>
</tr>
<tr>
<td>IL-MSE08</td>
<td>Mitsuhiro MATSUMOTO</td>
<td>Kyoto Univ.</td>
<td>Large-Scale MD Simulation of Mass and Heat Transfer at Interfaces</td>
</tr>
<tr>
<td>IL-MSE09</td>
<td>Nobuyuki MATUBAYASI</td>
<td>Kyoto Univ.</td>
<td>Free-Energy Calculation in Solution with the Method of Energy Representation</td>
</tr>
<tr>
<td>IL-MSE10</td>
<td>Shinichi MIURA</td>
<td>IMS &amp; GUAS, Okazaki</td>
<td>Path Integral Hybrid Monte Carlo Study of Solvated Molecules in Superfluid Helium-4 Clusters</td>
</tr>
<tr>
<td>IL-MSE11</td>
<td>Haruki NAKAMURA</td>
<td>Osaka Univ.</td>
<td>Computing Grid towards Multi-Level / Multi-Scale Biological Simulations</td>
</tr>
<tr>
<td>IL-MSE12</td>
<td>Iwao OHMINE</td>
<td>Nagoya Univ.</td>
<td>Water Dynamics; Potential Energy Landscape and Fluctuation</td>
</tr>
<tr>
<td>IL-MSE13</td>
<td>Yuko OKAMOTO</td>
<td>Nagoya Univ.</td>
<td>Nanosimulation of Protein Folding</td>
</tr>
<tr>
<td>IL-MSE14</td>
<td>Grenfel N. PATEY</td>
<td>Univ. of British Columbia</td>
<td>Forces and Structure in Nematic-Colloid Dispersions</td>
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<tr>
<td>IL-MSE15</td>
<td>B. Montogomery PETTITT</td>
<td>Univ. of Houston</td>
<td>Hydrophobic Association of Baroscopic Solutes</td>
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<tr>
<td>IL-MSE16</td>
<td>Peter J. ROSSKY</td>
<td>Univ. of Texas at Austin</td>
<td>Quantum Simulation of Molecular Clusters</td>
</tr>
<tr>
<td>IL-MSE17</td>
<td>James L. SKINNER</td>
<td>Univ. of Wisconsin</td>
<td>Computational Approaches to Vibrational Spectroscopy in Water: Line Shapes and Echoes</td>
</tr>
<tr>
<td>IL-MSE18</td>
<td>Hideki TANAKA</td>
<td>Okayama Univ.</td>
<td>Pase Behaviors of Confined Water</td>
</tr>
</tbody>
</table>
# List of Invited Speakers (Condensed Matter Theory (CMT))

<table>
<thead>
<tr>
<th>Code</th>
<th>Name</th>
<th>Affiliation</th>
<th>Topic</th>
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</thead>
<tbody>
<tr>
<td>IL-CMT01</td>
<td>Bernard BARBARA</td>
<td>Lab. Louis Neel-CNRS, Grenoble</td>
<td>Mesoscopic Physics with Rare-Earths</td>
</tr>
<tr>
<td>IL-CMT03</td>
<td>Nejat BULUT</td>
<td>Koç Univ., Istanbul</td>
<td>Magnetism and Superconductivity of Strongly Correlated Electrons (tentative)</td>
</tr>
<tr>
<td>IL-CMT04</td>
<td>James R. CHELIKOWSKY</td>
<td>Univ. of Texas at Austin</td>
<td>Magnetically Doped Quantum Dots</td>
</tr>
<tr>
<td>IL-CMT05</td>
<td>Toshiyuki KOYAMA</td>
<td>Nat. Inst. for Materials Sci., Tsukuba</td>
<td>Modeling of Complex Microstructure Changes in Metallic Materials Using the Phase-Field Method</td>
</tr>
<tr>
<td>IL-CMT06</td>
<td>Steven G. LOUIE</td>
<td>Univ. of California at Berkeley</td>
<td>Theory and Computation of the Optical, Transport, and Mechanical Properties of Nanostructures</td>
</tr>
<tr>
<td>IL-CMT07</td>
<td>Fernando LUIS</td>
<td>CSIC-Univ. de Zaragoza</td>
<td>Quantum and Classical Nonlinear Susceptibilities of Nanomagnets</td>
</tr>
<tr>
<td>IL-CMT08</td>
<td>Keiichiro NASU</td>
<td>Inst. of Materials Structure Sci., KEK, Tsukuba</td>
<td>Photogeneration of Ferroelectric and Conductive Nano Domain in SrTiO₃</td>
</tr>
<tr>
<td>IL-CMT09</td>
<td>Shuji OGATA</td>
<td>Nagoya Inst. of Tech.</td>
<td>Hybrid Quantum-Classical Simulation Over the Pacific Grid</td>
</tr>
<tr>
<td>IL-CMT10</td>
<td>Peter PRELOVSEK</td>
<td>Jozef Stefan Inst., Ljubljana</td>
<td>Finite-Temperature Dynamics in Microscopic Model for Cuprates: Small-System Results</td>
</tr>
<tr>
<td>IL-CMT11</td>
<td>Sandro SORELLA</td>
<td>SISSA, Trieste</td>
<td>Quantum Monte Carlo for Strongly Correlated Electrons (tentative)</td>
</tr>
<tr>
<td>IL-CMT12</td>
<td>Yasutami TAKADA</td>
<td>Univ. of Tokyo</td>
<td>Dynamical Properties of the Electron Liquid: Importance of the Excitonic Effect</td>
</tr>
<tr>
<td>IL-CMT13</td>
<td>Wolfgang WERNSDORFER</td>
<td>Lab. Louis Neel-CNRS, Grenoble</td>
<td>Quantum Dynamics in Single-Molecule Magnets</td>
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# List of Keynote Speakers

<table>
<thead>
<tr>
<th>Code</th>
<th>Name</th>
<th>Affiliation</th>
<th>Topic</th>
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<tbody>
<tr>
<td>KL01</td>
<td>Sadamichi MAEKAWA</td>
<td>Tohoku Univ.</td>
<td>Progress Report of the Group of Nano-Electron Systems - Electronic States in Strongly Correlated Systems -</td>
</tr>
<tr>
<td>KL02</td>
<td>Fumiyasu MIZUTANI</td>
<td>IMS, Okazaki</td>
<td>Grid Computing Management</td>
</tr>
<tr>
<td>KL03</td>
<td>Shigeru NAGASE</td>
<td>IMS &amp; GUAS, Okazaki</td>
<td>Functional Nanomolecule</td>
</tr>
<tr>
<td>KL04</td>
<td>Susumu OKAZAKI</td>
<td>IMS &amp; GUAS, Okazaki</td>
<td>Molecular Dynamics and Statistical Mechanical Studies on Structure and Dynamics of Nano-Scale Molecular Assemblies in Solution by NAREGI Nanoscience Project</td>
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<tr>
<td>KL05</td>
<td>Hajime TAKAYAMA</td>
<td>Univ. of Tokyo</td>
<td>Nano-Magnetism</td>
</tr>
<tr>
<td>KL06</td>
<td>Kiyoyuki TERAKURA</td>
<td>AIST, Tsukuba</td>
<td>Nano-System Designing</td>
</tr>
</tbody>
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