

MASP2012

ISSP-CMSI
International Workshop
Material Simulation in Petaflops era

MASP2012 is the sixth of ISSP workshop/symposium on theoretical physics since 2006. This meeting will focus on the first-principles electronic structure calculations related to the energy and environment research. Anticipated topics of discussion include:

- (1) Dispersion force and hydrogen bound
- (2) Excited state, dissipation, and superconductivity
- (3) Accurate and/or large-scale ground state calculations
- (4) Application to energy-conversion processes --- photocatalysis, fuel cells and solar cells

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|--------|---------------------------------------------------------------------------------------------------|
| Date: | [Workshop] June 25 (M) - July 1st (Su) July 3 (Tu) - 11 (W), 2012 |
| | [Symposium] July 2 (M), 12 (Th), 13 (F), 2012 |
| Venue: | The University of Tokyo Kashiwa Campus [Workshop] Kashiwa Lib. Seminar Rm. & Conference Rm. |
| | [Symposium] IPMU Lecture Hall (July 2) Kashiwa Lib. Media Hall (July 12, 13) |

Invited Speakers (from abroad)

(A) van der Waals interaction

- O. A. von Lilienfeld** (Argonne National Laboratory, USA)
J. Dobson (Griffith University, Australia)

(B) excited state, dissipation, and superconductivity

- M. Rohlfing** (University of Osnabrück, Germany)
E. K. U. Gross (Max Planck Inst. of Microstructure Physics, Germany)
A. Marini (National Research Council, Italy)
M. Di Ventra (University of California, USA)

(C) quantum monte carlo approach

- L. Mitas** (North Carolina State University, USA)
N. Marzari (École Polytechnique Fédérale de Lausanne, Switzerland)

(D) simulation at the interface

- M. Sprik** (Cambridge University, UK)
T. Ogitsu (Lawrence Livermore National Laboratory, USA)
M. Björketun (Technical University of Denmark, Denmark)
M. Koper (Leiden University, Netherlands)
J. Vande Vondele (Eidgenössische Technische Hochschule Zürich, Switzerland)

(E) large scale simulation

- F. Gygi** (University of California, USA)

Organising Committees

S. Tsuneyuki, K. Yamashita (U. Tokyo) T. Ohno, Y. Tateyama (NIMS) Y. Miyamoto (AIST)
N. Kawashima, H. Noguchi, Y. Noguchi, O. Sugino* (ISSP, U. Tokyo) *Chair



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