

Cooperation of Computational Materials Science and Mathematics toward Smart Materials Design II

— What Materials Informatics brings in? —

http://www.wpi-aimr.tohoku.ac.jp/mathematics_unit/coop-mathworkshop/

Study Group : January 6th (Mon.) - 7th (Tue.), 2014

Place : JST Tokyo Headquarters. K's Gobancho (7, Gobancho, Chiyoda-ku, Tokyo, 102-0076 Japan)

Workshop : January 8th (Wed.) - 9th (Thu.), 2014

Place: WPI-AIMR, Tohoku University 2nd Floor Seminar Room (2-1-1 Katahira, Aoba-ku, Sendai, 980-8577 Japan)

Program

January 6th : Study Group

- 10:00 **Isao Tanaka** (Kyoto University)
"OPENING"
- 10:15-12:00 **Krishna Rajan** (Iowa State University)
"MATERIALS INFORMATICS: PRINCIPLES AND APPLICATIONS"
— I. Mapping and Systematics of Materials Data —
- 13:30-15:00 **Krishna Rajan** (Iowa State University)
"MATERIALS INFORMATICS: PRINCIPLES AND APPLICATIONS"
— II. Elements of Data Mining —
- 15:30-17:00 **Short presentations**
Tetsuo Mohri (Tohoku University), **Kazuto Akagi** (Tohoku University), **Shinji Tsuneyuki** (University of Tokyo)

January 7th : Study Group

Coordinator : **Kenji Fukumizu** (Institute of Statistical Mathematics)

- 9:30-12:00 **Ryo Yoshida** (Institute of Statistical Mathematics)
"Bayesian Statistics for Data Assimilation"
- 13:30-15:00 **Krishna Rajan** (Iowa State University)
"MATERIALS INFORMATICS: PRINCIPLES AND APPLICATIONS"
— III. Applications and Case Studies —
- 15:30-17:00 **Discussions**, Chair **Motoko Kotani** (Tohoku University)
"Mathematical Challenge to Materials Informatics- How we enhance Materials Science in Japan"

January 8th : Workshop

- 13:30-15:10 **Masato Okada** (University of Tokyo)
"Bayesian spectral deconvolution and sparse modeling"
- 15:20-16:10 **Shinji Saito** (Institute for Molecular Science)
"Spatio-temporal heterogeneous dynamics in condensed phases"
- 16:30-17:20 **Krishna Rajan** (Iowa State University)
"Data Dimensionality and Data Topology in Materials Science"

Discussions

Party @ Restaurant "Hagi"

January 9th : Workshop

- 10:00-10:50 **Koji Hukushima** (University of Tokyo)
"Inference of an effective physical model from STM imaging data :
an example of data-driven science in condensed matter physics"
- 11:00-11:20 **Takenobu Nakamura** (Tohoku University)
"A characterization of the amorphous silica structure by persistent homology"
- 11:30-11:50 **Chihiro Nakajima** (Tohoku University)
"Reconstruction of the 3D structure of the nanocrystals using Monte Carlo method"
- 12:00-12:20 **Natsuhiko Yoshinaga** (Tohoku University)
"Dynamics of *shape* in nonequilibrium soft materials"
- 14:00-14:50 **Tetsuo Mohri** (Tohoku University)
"First-principles multiscale calculations for microstructure evolution process"