

International Workshop of Materials Informatics and Materials Data (MIMD)

6th-7th April 2017, Tsukuba, Japan

Venue: Conference Room#2, 1st Floor, Main Bldg. NIMS Sengen site

The purpose of this workshop is to promote communication and collaboration between researchers in different countries in the field of materials informatics and materials data. The most current research topics and results in the institutions of China, Germany and Japan will be presented.

Program

| Day 1 (Apr. 6 th , Thu.) | |
|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------|
| Registration | 12:30- |
| Opening | 13:00-13:10 |
| • "Solute concentrations and strains in nanograined materials and nanoparticles" Tong-Yi Zhang (SHU, China) | 13:10-14:10 |
| • "Multiple Genomes for Catalytic Performance of Zeolite" Yi Liu (SHU, China) | 14:10-14:50 |
| • "Liquid electrolyte material search for Li-ion batteries" Keitaro Sodeyama (NIMS, Japan) | 14:50-15:30 |
| Break | 15:30-15:45 |
| • "Thermal conductivity and lattice anharmonicity from first principles : Theoretical developments and applications" Terumasa Tadano (NIMS, Japan) | 15:45-16:25 |
| • "A compressive-sensing approach to finding physically meaningful descriptors from materials data" Sergey V. Levchenko (FHI, Germany) | 16:25-17:05 |
| Day 2 (Apr. 7 th , Fri.) | |
| Registration | 9:30- |
| • "Materials database and data integration" Quan Qian (SHU, China) | 10:00-10:40 |
| • "Using support vector machine for materials design and optimization" Wencong Lu (SHU, China) | 10:40-11:20 |
| • "Inverse design of functional materials: advanced machine learning techniques coupled to computational experiments" Guillaume Lambard, Stephen Wu, Ryo Yoshida (ISM, Japan) | 11:20-12:00 |
| Lunch | 12:00-13:00 |
| • "Integrated computational thermodynamics and database " Xiaogang Lu (SHU, China) | 13:00-13:40 |
| • "Calphad and its role in MI2" Taichi Abe (NIMS, Japan) | 13:40-14:20 |
| Break | 14:20-14:35 |
| • "High throughput material synthesis for energy related materials research" Masahiro Goto (NIMS, Japan) | 14:35-15:15 |
| • "Thermal transportation at interface: experimental, theoretical and data science approaches" Yibin Xu (NIMS, Japan) | 15:15-16:00 |
| Closing | 16:00-16:10 |

Organized by

Center for Materials Research by Information Integration, National Institute for Materials Science, Japan
Materials Genome Institute, Shanghai University, P.R. China

