

Summary of the e-ASIA JRP Online Workshop on "Materials Informatics"

Co-organized by

Agency for Science, Technology and Research (A*STAR),

Japan Science and Technology Agency (JST),

and e-ASIA JRP Secretariat.

Supported by

Program Management Unit for Human Resources & Institutional Development, Research and Innovation (PMU-B),

National Science and Technology Development Agency (NSTDA),

and Department of Science and Technology (DOST).

13-14 January, 2021

Overview



Workshop Theme

- ✓ Materials Informatics
- **Focus Topics**
 - ✓ Materials platforms and tools
 - ✓ Materials informatics for alloy development and processing
 - ✓ Materials informatics for a low-carbon society

Participants

 ✓ 92 participants including 28 invited speakers (Singapore, Japan, Thailand, Philippines, Indonesia)

Background



Rapid expansion of Materials Informatics (MI)

Due to:

✓ The advancement of computers and information processing technology in recent years.

✓ The application of computer technology to materials science research.

Many New initiatives relating to MI

- ✓ in Japan, Europe and the United States,
- ✓ in Southeast Asia

Objectives



✓ Discuss hot topics of "Materials Informatics" as the most advanced materials research field, among cutting-edging researchers from Japan, Singapore, Thailand, and Philippines.

- ✓ Establish a tight researchers' network among participants for better international collaboration.
- ✓ Explore potential collaboration opportunities to prepare for the e-ASIA JRP 10th joint call on "Materials Informatics".

Agenda



Opening Remarks

✓ **Prof. Andy Hor**, Deputy Chief Executive (Research), Agency for Science Technology and Research (A*STAR)

✓ **Dr. Osamu Aruga,** Director, Ministry of Education, Culture, Sports, Science and Technology (MEXT)

Keynote Speech

✓ Prof. Teruo Kishi, Program Director,
Japan Science and Technology Agency



Agenda



Technical Sessions

- ✓ Materials platforms and tools (10 invited talks)
- ✓ Materials informatics for alloy development and processing (10 invited talks)
- ✓ Materials informatics for a low-carbon society (10 invited talks)

Group Discussion and Wrap-up Session

✓ Build international joint research teams for future collaboration, preparing for the e-ASIA JRP call of "Materials Informatics".

Comments from Advisor / Co-organizer

- ✓ **Prof. Teruo Kishi,** Program Director, Japan Science and Technology Agency
- ✓ Dr. You Huan Yeo, Director, International Operations and Relations Office, A*STAR

Agenda



Presentation from RIKEN representatives

- ✓ **Prof. Satoshi Matsuoka,** Director, RIKEN Center for Computational Science
- ✓ Dr. Takahito Nakajima, Team Leader, RIKEN Center for Computational Science

Comments from the e-ASIA call participating funding agencies

✓ Japan: JST (Mr. Osamu Kobayashi, Director, International Affairs, Japan Science and Technology Agency)

✓ Philippines: DOST (Dr. Enrico C. Paringit, Executive Director, Philippine Council for Industry, Energy, and Emerging Technology Research and Development (DOST-PCIEERD))

✓ **Singapore: A*STAR (Dr. Michael Sullivan,** Department Director, A*STAR Institute of High Performance Computing)

✓ **Thailand: PMU-B (***Dr.Kanyawim Kirtikara,* Executive Director, Program Management Unit for Human Resources & Institutional Development, Research and Innovation)



B



Photos (Technical Session, Group Discussion)

Session1

































Session3



and 1 NSTOA





























Conclusions

Common Research Interest in Materials Informatics

 ✓ Materials development in alloys via techniques in Materials Informatics & Materials Integration.

- ✓ Alloy Design from High-Throughput DFT & Machine-learning Models.
- ✓ Alloy Designing over multi spatio-temporal scales.
- ✓ Advanced simulation and Data science of Alloy development for the further research.
- ✓ Materials informatics approaches, in conjunction with high-throughput calculations or high-throughput experiments, for a low-carbon society.

Conclusions

Possible Collaboration Projects

✓ Develop novel correlations between nanoscale properties and mesoscale properties and use this correlation to screen for promising new alloys.

- ✓ Incorporation of nanoscale materials in bulk engineering alloys for improved properties.
- ✓ Design "dual-use" alloys that have both excellent functional and structural properties (e.g., magnetic alloys with good structural properties and corrosion resistance).
- ✓ Digital Twin: Advanced modelling & simulation of AM (additive manufacturing).
- ✓ Mechanical property prediction (crystal plasticity, machine learning, AI).
- ✓ Thermoelectric/thermal conductivity materials (Material search to process).
- ✓ Battery materials & systems (Material search and analytics for degradation).
- ✓ Catalyst materials (Material search and manufacturing).

Thank you for your strong support to e-ASIA joint Research Program.