e-ASIA Joint Research Program 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)

Date: January 13th and 14th, 2021

Workshop Agenda

January 13th (Wednesday)

Time	Program
(Singapore)	
7:45 – 8:00	Workshop Opens
Opening Session	
MC (Dr. Michael S	Sullivan, Department Director, A*STAR Institute of High
Performance Com	puting)
8:00 - 8:05	Opening Remarks
	Prof. Andy Hor, Deputy Chief Executive (Research), Agency for
	Science Technology and Research (A*STAR)
8:05 – 8:10	Opening Remarks
	Dr. Osamu Aruga, Director, Ministry of Education, Culture,
	Sports, Science and Technology (MEXT)
8:10 – 8:25	Keynote Speech
	Prof. Teruo Kishi, Program Director, Japan Science and
	Technology Agency
8:25 - 8:30	Group Photo
Technical Sessio	ns
< Objectives >	
Discuss issues and concerns in the topic area, and potential solutions.	
Prepare observations and recommendations for workshop wrap-up.	
Develop project ideas and possibility of joint research activities.	
< Time allotted to each speaker >	
20 minutes each for presentation	
- Session 1: Materials platforms and tools -	

8:30 - 8:40	Speaker 1-1
	Introduction (overview)
	Prof. Tetsuo Mohri, Professor Emeritus, Hokkaido University,
	Japan
8:40 - 8:50	Speaker 1-2
	Introduction (overview)
	Dr. Teck Leong Tan, Deputy Department Director, A*STAR
	Institute of High Performance Computing, Singapore
Presentation	Speech 15min. Q&A 5min. for each presentation
8:50 – 9:10	Speaker 1-3
	Dr. Takashi Miyake, Research team leader, The National
	Institute of Advanced Industrial Science and Technology (AIST),
	Japan
	"Data-driven materials design of high-performance
	permanent magnets"
9:10 - 9:30	Speaker 1-4
	Dr. Teck Leong Tan, Deputy Department Director, A*STAR
	Institute of High Performance Computing, Singapore
	"Alloy Design via High-Throughput DFT & Machine-learned
	Surrogate Models"
9:30 - 9:50	Speaker 1-5
	Prof. Manabu Enoki, Professor, University of Tokyo, Japan
	"Design of Structural Materials by Data-driven Approach in
	Materials Integration Project"
9:50 - 10:10	Speaker 1-6
	Dr. Mark Jhon, Senior Scientist, A*STAR Institute of High
	Performance Computing, Singapore
	"Multiscale modeling for Designing and Understanding
	Length Scale Effects in Allovs"
10.10 - 10.30	Speaker 1-7
	Prof. Masao Takevama . Professor. Tokvo Institute of
	Technology, Japan
	"Integrated Inverse Design Approach to Development of
	Innovative Powder Processed TiAl Alloys for Jet Engine
	Application"
10:30 - 10:50	Speaker 1-8
	Prof. Yuan Ping Feng, Professor, National University of
	Singapore, Singapore
	"2DMatPedia: A Library of 2D Materials and Screening of
	Magnetic Electrenes"
10:50 - 11:10	Speaker 1-9

	Dr. Manaschai Kunaseth, Research team leader, NSTDA
	Supercomputer Center, Thailand
	"Thailand's HPC infrastructure readiness for emerging
	computational materials science and informatics"
11:10 – 11:30	Speaker 1-10
	Dr. Chanchana Thanachatanont, Director of Environment
	Research Group, National Metal and Materials Technology
	Center, Thailand
	"Determination of pesticides in water using hybrid-material-
	modified electrodes and data analytics"
11:30 – 12:30	Session 1 Group Discussion on future collaboration
	opportunities in e-ASIA JRP
	Each session-chair will lead their discussion and prepare a short
	presentation for wrap-up.
12:30 - 13:00	Lunch Break
Section 2: M	starials information for allow development and processing
- 36351011 2. 141	atenais informatics for alloy development and processing -
13:00 – 13:10	Speaker 2-1
	Introduction (overview)
	Prof. Makoto Watanabe, Field Director, National Institute for
	Materials Science; Adjunct professor, Shibaura Institute of
	Technology, Japan
13:10 – 13:20	Speaker 2-2
	Introduction (overview)
	Dr. Sharon Nai, Deputy Division Director, Senior Scientist,
	A*STAR Singapore Institute of Manufacturing Technology,
	Singapore
Presentation	Speech 15min. Q&A 5min. for each presentation
13:20 – 13:40	Speaker 2-3
	Prof. Yuichiro Koizumi, Professor, Osaka University, Japan
	"Computer Simulations for Creating Digital Twin of Powder
	Bed Fusion (PBF) type Additive Manufacturing (AM):Toward
	Site-Specific Microstructure Engineering"
13:40 - 14:00	Speaker 2-4
	Dr. Dennis Tan, Deputy Head, A*STAR Institute of Materials
	Research and Engineering, Singapore
	"Iterative Combinatorial Approach to Alloy Development:
	augmenting with compositionally graded AM fabrication
	and high-throughput screening"
14:00 - 14:20	Speaker 2-5

	Prof. Naoyuki Nomura, Professor, Tohoku University, Japan
	"Challenges of composite powder fabrication for additive
	manufacturing"
14:20 - 14:40	Speaker 2-6
	Dr. Guglielmo Vastola, Scientist, A*STAR Institute of High
	Performance Computing, Singapore
	<i>"IHPC's 'Digital Twin" platform for additive manufacturing:</i>
	an integrated multiscale high-fidelity simulation of powder-
	bed fusion and directed energy deposition additive
	manufacturing"
14:40 - 15:00	Speaker 2-7
	Dr. Sharon Nai, Deputy Division Director, Senior Scientist,
	A*STAR Singapore Institute of Manufacturing Technology,
	Singapore
	"Tailoring AM printable materials and components for
	lightweight and superior performance: design, process-
	microstructure-performance mapping"
15:00 – 15:20	Speaker 2-8
	Dr. Tongjai Chookajorn, Scientist, National Metal and Materials
	Technology Center, Thailand
	"Inermodynamics-based Monte Carlo calculation of alloy
15.20 15.40	Structures
15.20 - 15.40	Dr Allan Abraham Padama Associate Professor University of
	the Dhilippines Lee Bones, Dhilippines
	"Rehavior of Birnstellin Ostalista in the Brassnes of
	"Benavior of Bimetallic Catalysts in the Presence of
	Adsorbates: Insights from Atomistic Calculations and the
	Possible Application of Materials Informatics"
15:40 – 16:00	Speaker 2-10
	Prof. Junya Inoue , Associate Professor, University of Tokyo,
	Japan "O
	"Sparse modeling for understanding process-structure-
16:00 17:00	property linkage"
10:00 - 17:00	Session 2 Group discussion on future collaboration opportunities in a
	Fach session-chair will lead their discussion and prepare a short
	presentation for wrap-up

January 14th (Thursday)

Time (Singapore)	Program
8:15 – 8:30	Workshop Opens
- Session 3: Materials informatics for a low-carbon society -	
8:30 - 8:45	Speaker 3-1
	Introduction (overview)
	Prof. Kohei Uosaki, Fellow and Executive Advisor to the
	President, National Institute for Materials Science; Professor
	Emeritus, Hokkaido University, Japan
	Prot. Yoshitaka Tateyama, Group leader, National Institute for
9.45 0.00	Materials Science, Visiting Professor, Waseda University, Japan
0.45 - 9.00	Speaker 3-2
	Dr. Zhi Wei Seh , Senior Scientist, A*STAR Institute of Materials
	Research and Engineering, Singapore
Presentation	Speech 15min. Q&A 5min. for each presentation
9:00 - 9:20	Speaker 3-3
	Dr. Randy Jalem, Senior Researcher, National Institute for
	Materials Science, Japan
	"Computational design and exploration of novel solid
	electrolytes for all-solid state batteries by DFT and machine
	learning"
9:20 - 9:40	Speaker 3-4
	Dr. Edwin Khoo, Research Scientist, A*STAR Institute for
	Infocomm Research, Singapore
	"Scientific machine learning for battery analytics"
9:40 - 10:00	Speaker 3-5
	Dr. Yibin Xu, Deputy Director, National Institute for Materials
	Science, Japan
	"Application of Materials Informatics to Interface
	Engineering of Energy Materials"
10:00 – 10:20	Speaker 3-6
	Prof. Kedar Hippalgaonkar, Assistant Professor, Nanyang
	Technological University, Singapore
	"Accelerated Materials Development with Machine Learning,
	High Performance Computing and Automated Laboratories –
	design of functional materials"
10:20 – 10:40	Speaker 3-7
	Prof. Panida Surawatanawong, Associate Professor, Mahidol
	University, Thailand

	<i>"Mechanisms of H2 Activation and C-O Activation: Metal Cooperative Lewis Pairs"</i>
10:40 - 11:00	Speaker 3-8
	Prof. Junya Hasegawa, Professor, Hokkaido University, Japan
	"Catalyst Informatics Cooperation among Institutes in
	Japan"
11:00 – 11:20	Speaker 3-9
	Dr. Yee-Fun Lim, Senior Scientist, A*STAR Institute of Materials
	Research and Engineering, Singapore
	"Accelerated Catalyst Development Platform"
11:20 – 12:20	Session 3
	Group Discussion on future collaboration opportunities in e-
	ASIA JRP
	Each session-chair will lead their discussion and prepare a short
	presentation for wrap-up.
12:20 - 13:00	Lunch Break

Wrap-up Session on Potential Future Collaboration under the e-ASIA JRP	
(MC: Emi Kaneko, Director, JST Singapore office, Japan)	
13:00 – 13:20	Information of e-ASIA 10 th Call on "Materials informatics and advanced material research by utilizing computers" <i>e-ASIA JRP Program Secretariat</i>
13:20 – 13:50	 Presentation from RIKEN representatives Prof. Satoshi Matsuoka, Director, RIKEN Center for Computational Science "Overview of Fugaku: the First Exascale Supercomputer and its Fight Against COVID-19" Dr. Takahito Nakajima, Team Leader, RIKEN Center for Computational Science "Materials informatics and simulation on supercomputers"
13:50 – 14:30	 Wrap-up Presentation and Comments Each session chair to present a short summary of the group discussion. 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
Closing Session	

14:30 – 14:45	Comments from the e-ASIA call participating funding agencies (by the alphabetical order of country)
	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)
End of the Workshop	