

Overview of the Outcomes from
**e-ASIA JRP International Workshop
on Materials Informatics**

Session 1: Materials platforms and tools

Chairs:

**Prof. Tetsuo Mohri
Professor Emeritus, Hokkaido University**

**Dr. Teck Leong Tan
Deputy Department Director, A*STAR Institute of High
Performance Computing**

session 1 Materials platforms and tools

Application

- Design of functional alloys, Permanent magnets, electrocatalysts
- Design of structural alloys, including steels, Al alloys and TiAl alloys (for aerospace applications)
- Design of alloy nanoparticles
- Application to sensing of pesticides in water
- Screening of magnetic 2D electrenes

Tools and Method

(Machine learning)

- Machine learning
- Data assimilation technique
- Bayesian optimization
- Principal component Analysis (PCA)
- Artificial Neural Networks (ANN)

(Computation)

- First-principles calculation
- Monte Carlo simulation
- Finite element simulation

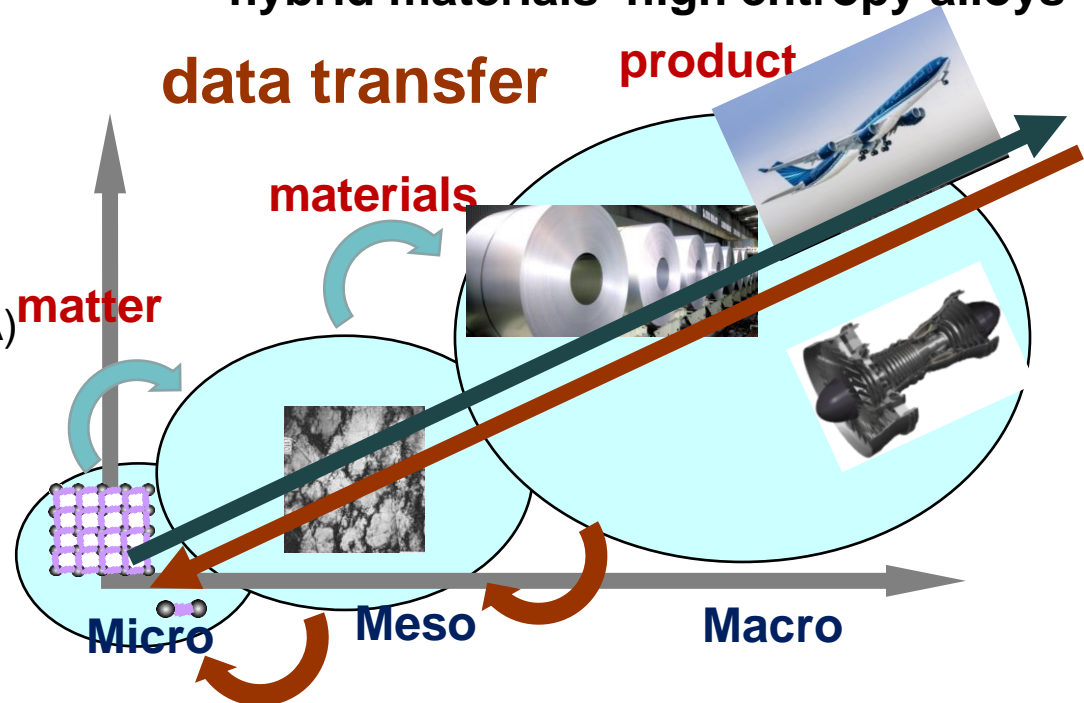
(Experiment)

- SEM, TEM, XRD...

Platforms and database

- SIP in Japan
- National HPC infrastructure in Thailand (ThaiSC)
- Open Quantum Materials DB (OQMD),
- 2D MatPedia

Interface boundary etc
hybrid materials high entropy alloys



Proposed Research Themes and Partners (Session 1)

Proposed Themes:

Platform for alloy design combining two or more approaches from Materials Informatics and Materials Integration techniques.

Possible examples include (but not limited to):

- 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).**

Prospective Partners:

-Singapore, Japan, Thailand, Philippines, Indonesia

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**Session 2: Materials informatics for alloy
development and processing**

Chairs:

Prof. Makoto Watanabe
Field Director, National Institute for Materials Science

Dr. Sharon Nai
Deputy Division Director, Senior Scientist, A*STAR
Singapore Institute of Manufacturing Technology

Towards Multilateral Collaboration on Session 2

Subtopics

- Materials informatics for alloy development and processing (linking advanced processing data, characterization data to property prediction), includes additive manufacturing and corrosion.
- Design of alloys and processing for additive manufacturing, enhanced structural properties, corrosion resistance.

Target

- We will build international joint research teams for e-ASIA call.

Proposed Research Themes and Partners

(Session 2)

Proposed Themes:

- Digital Twin: Advanced modelling & simulation of AM
 - Collaboration opportunities of A*STAR simulation platform
 - Mechanical property prediction (crystal plasticity, machine learning, AI)
 - Grain refinement and microstructural control
 - Atomistic simulation
 - Understanding of crack formation mechanism & suppression methodology
 - New material powders & component level production
 - Composite powders
 - Alloy powders
- * Data sharing & target materials to be considered.*

Prospective Partners:

Singapore, Japan, Thailand and Philippines

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**Session 3: Materials informatics for a low-
carbon society**

Chairs:

Prof. Kohei Uosaki

**Fellow and Executive Advisor to the President, National
Institute for Materials Science**

Prof. Yoshitaka Tateyama

Group leader, National Institute for Materials Science

Dr. Zhi Wei Seh

**Senior Scientist, A*STAR Institute of Materials Research and
Engineering**

Towards Multilateral Collaborations in **Session 3**

<Summary>

Materials informatics approaches, in conjunction with high-throughput calculations or high-throughput experiments, for a low-carbon society were introduced in this session.

In particular, topics of battery materials, thermoelectric materials / materials with thermal conductivity, catalytic materials were selected for possible collaborations.

Not only understanding of & search for materials / surfaces / interfaces, but diagnosis, manufacturing & development platform have been targeted.

Examples:

Bayesian optimisation \leftrightarrow High-throughput Exp. or Materials search.

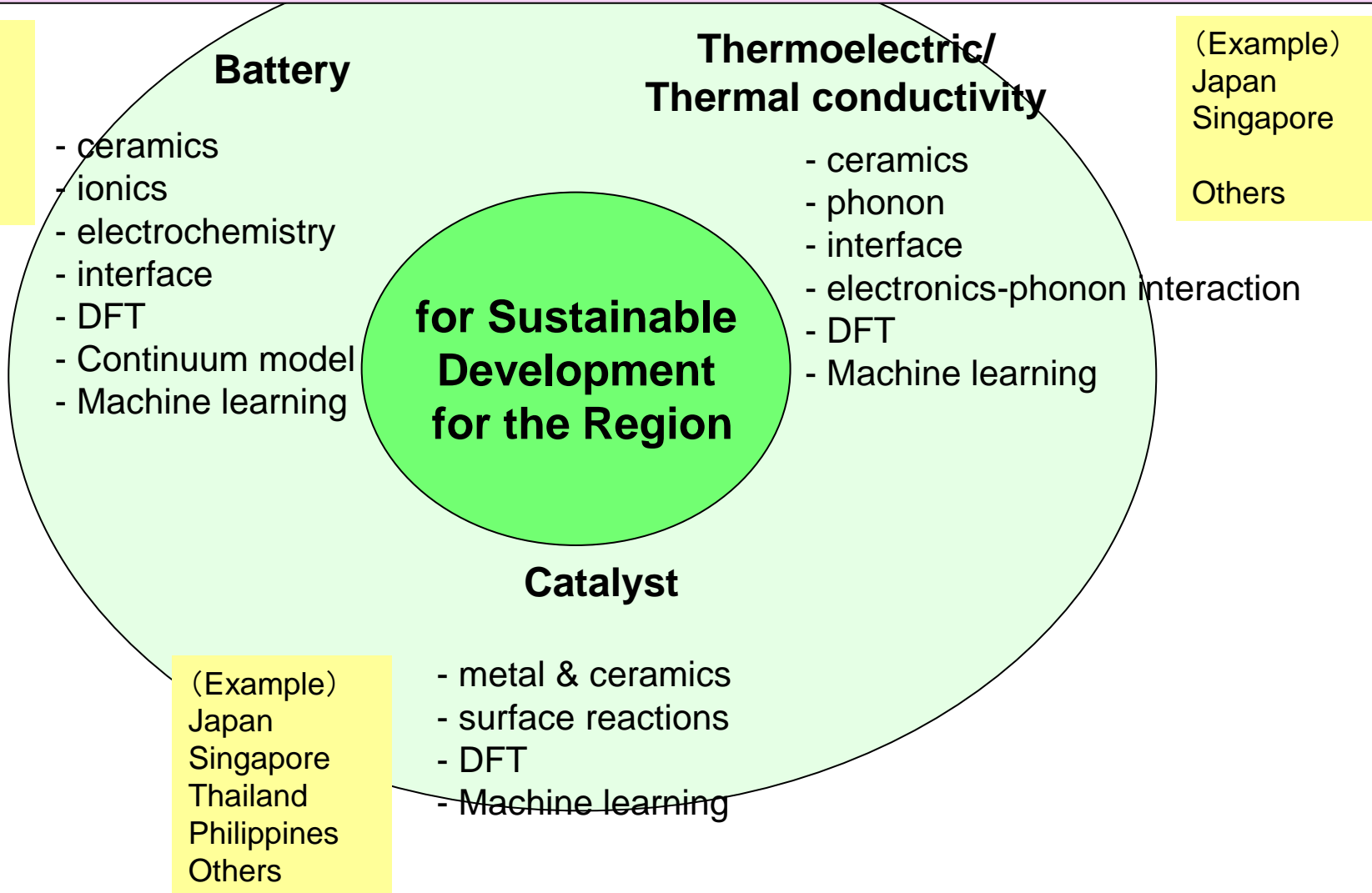
High-throughput DFT calculations \leftrightarrow Database expansion

Graph analysis, regression etc. in the Materials Informatics (MI) side

DFT, continuum model in the High-Performance Computing (HPC) side

Prospective Players in the Research Field

**Materials informatics for a low-carbon society
(including batteries, fuel cells, hydrogen, methane and thermoelectrics)**



Expected Research Themes and Partners

(Session 3)

1: Thermoelectric/thermal conductivity materials

Material search to process

2: Battery materials & systems

Material search and analytics for degradation

3: Catalyst materials

Material search and manufacturing

Expected Research Themes and Partners

(Session 3)

Grouping by the methods (key technologies):

HPC: DFT, MD, MC, kinetics

ML: Regression, Clustering, Neural Network (Potential)

Bayesian statistics/optimization, Pareto optimality → search

Diagonal combinations are also fine.

Finding other researchers for more specific topic is OK.

We are still flexible!

What can be expected from e-ASIA JRP Collaboration in **Session 3**

- **Synergistic, supplemental and leveraged effects by multilateral cooperation through joint funding**
 - **Novel knowledge and competitive technology**
 - **Genuine Partnerships for mutual contribution**
 - **Nurturing human resources through research collaboration and researchers' exchange**
- **Materials informatics for a low-carbon society and sustainability of the region**

Thank you for your attention

