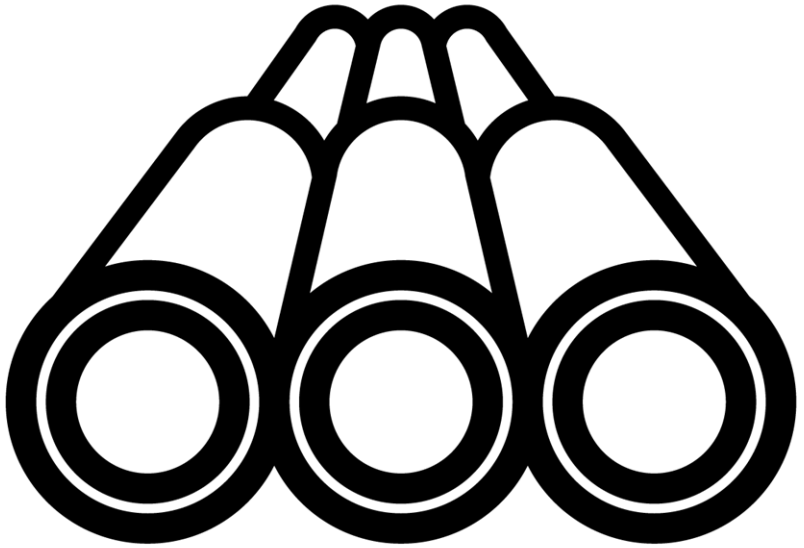
MEEP;
Materials Exploration space Extension Platform

(Materials Exploration Platform; Expanding Search Space by high-throughput technology)

HITOSUGI Taro
(TIT)



ONO Kanta
(Osaka Univ.)

USHIKU Hirotaka
(OSX)

CHIKYOW Toyohiro
(NIMS)

NAGATO Keisuke (Univ. Tokyo)

Outline

1. Background

1-1 Social Issues surrounding Materials R&D

1-2 Materials R&D problems in Japan

2. Factors and Measures

2-1 Extension of materials exploration space

2-2 ①Beyond human activity →HT autonomous systems

2-3 ②Beyond human knowledge→ Data-driven “Hybrid” method

2-4 ③Gather human knowledge → Knowledge sharing

3. Research contents

3-1 Research organization

3-2 Research plan

4. Summary

1. Background

1-1 Social issues surrounding Materials R&D

World issues

https://meti-journal.jp/p/13066-2/

Carbon Neutral 2050

https://www.keidanrensdgs.com/home-jp

SDGs

Corres pondece

Mater ials | Electronic Mater. | Ion conducting Mater. | Magnetic Mater. | Alternative Mater. | Structural Mater. | Circulating Mater. | Organic Mater. | Dielectric Mater.

Materials R&D is essential for the future society in the world

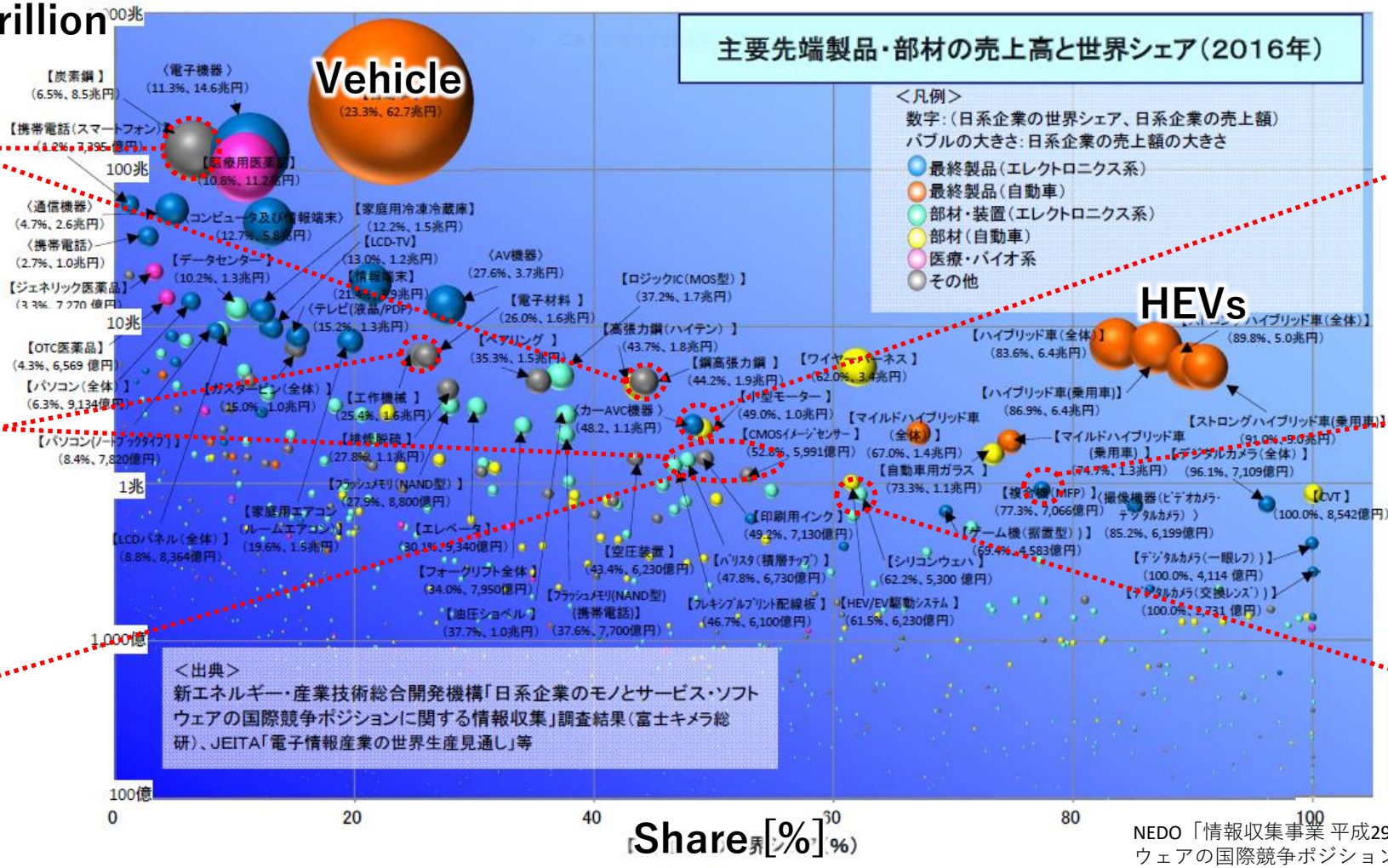
1. Background

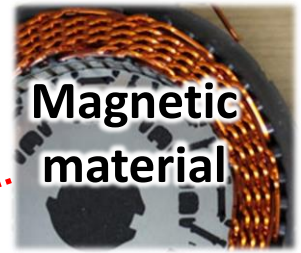
1-1 Social issues surrounding Materials R&D

Structural material

Electronic material

Dielectric material





Magnetic material

Organic material

Ion-conductive material

NEDO「情報収集事業 平成29 年度 日系企業のモノとサービス・ソフトウェアの国際競争ポジションに関する情報収集」、（2018年3月）

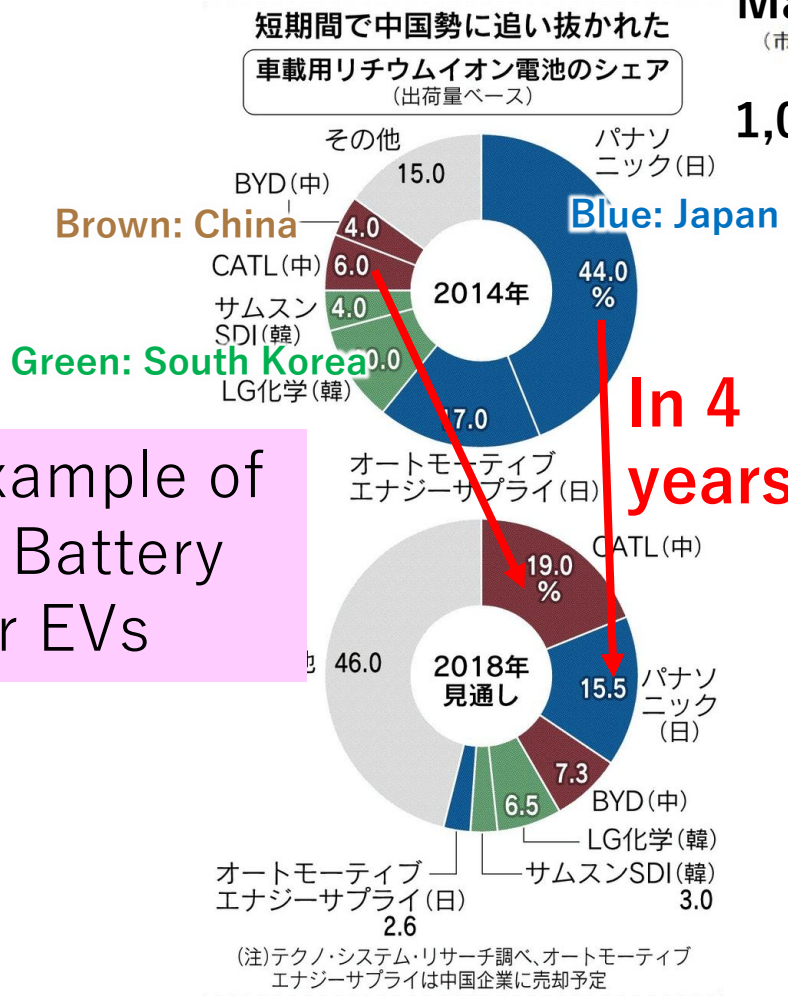
Materials industry is an important base of MONOZUKURI industry

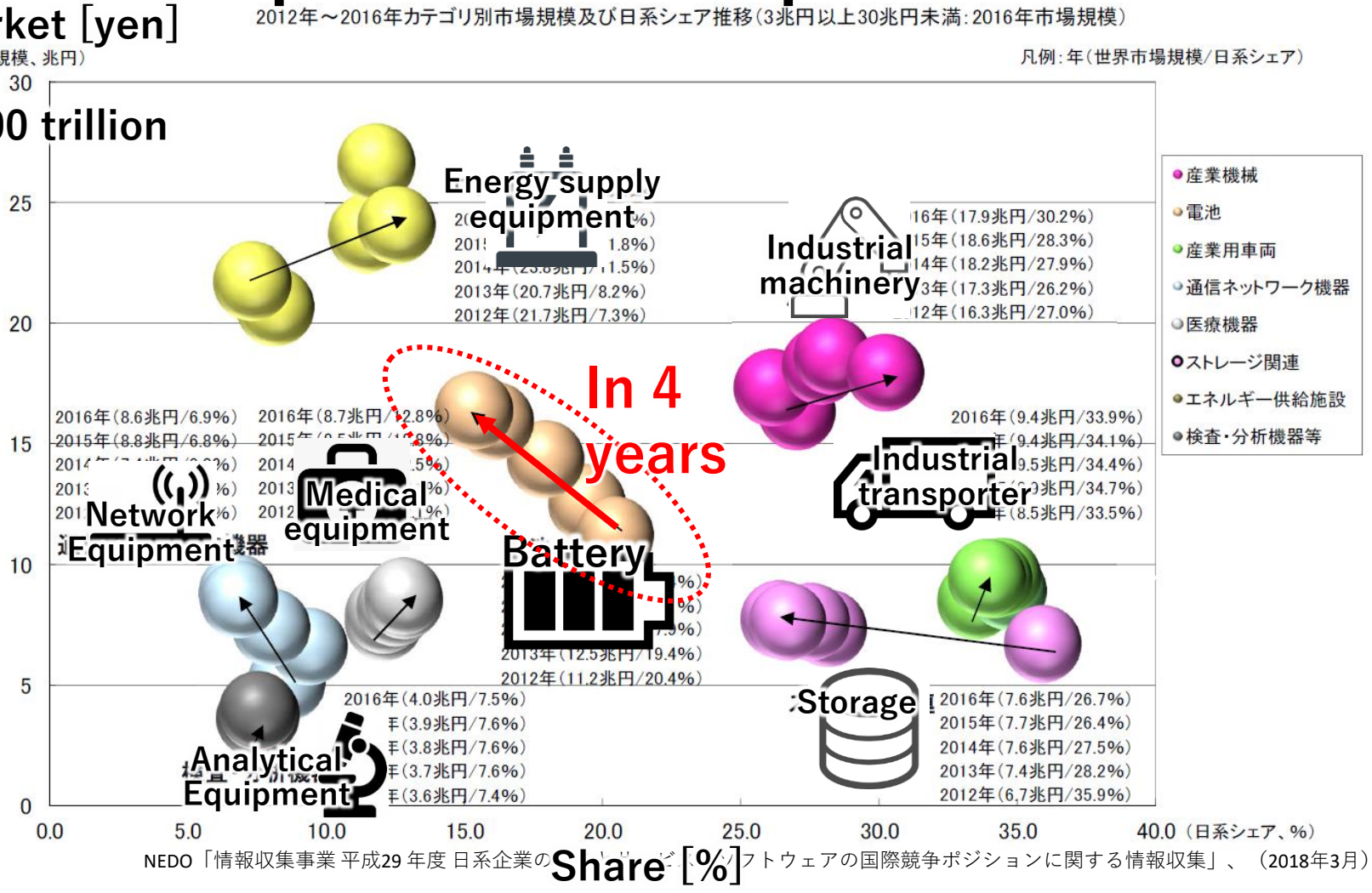
→ Materials R&D is more and more important

1. Background

1-2 Materials R&D problems in Japan

Example of Li Battery for EVs





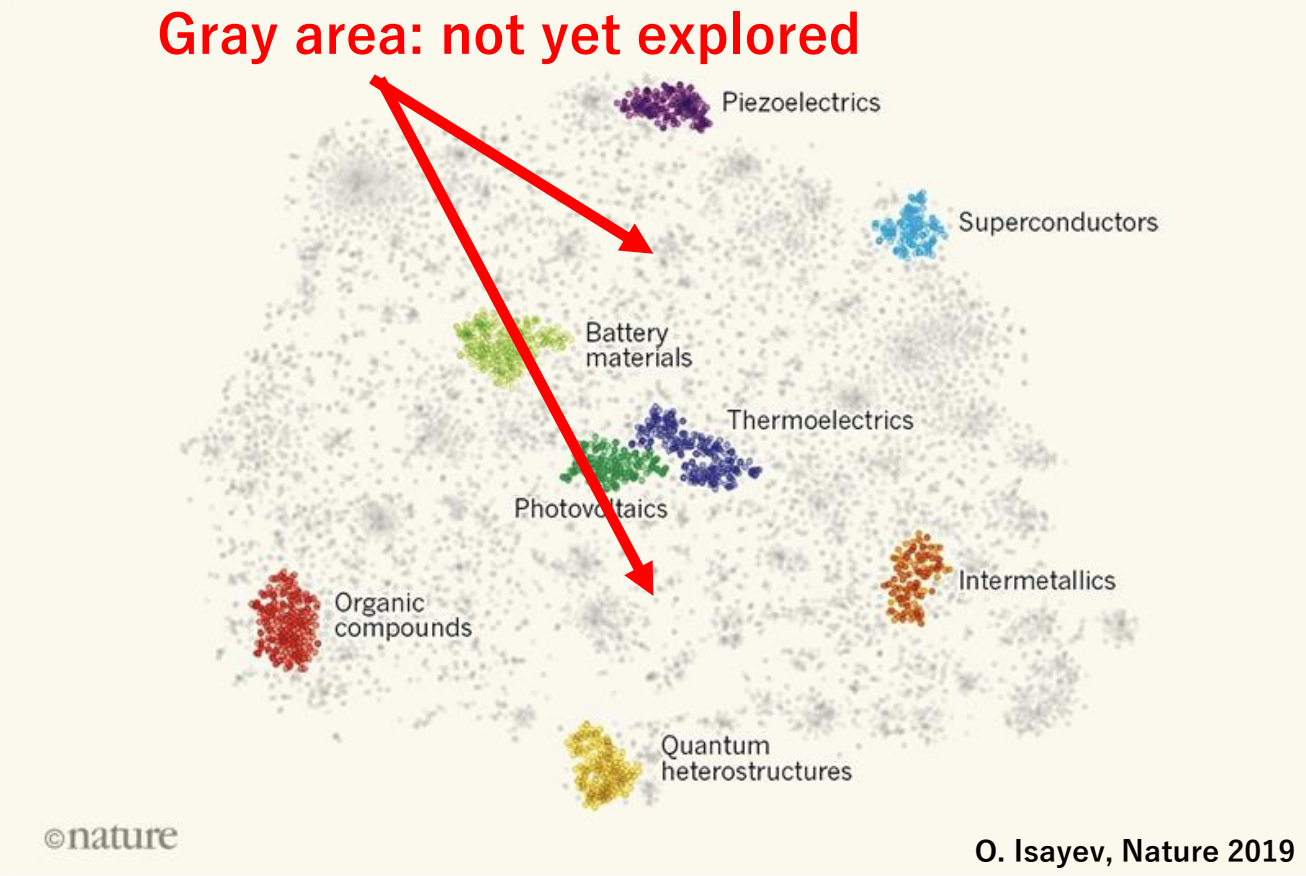
NEDO「情報収集事業 平成29 年度 日系企業の [illegible] フトウェアの国際競争ポジションに関する情報収集」、（2018年3月）

Industrial competitiveness is declining

How to achieve results?

1. Background

1-2 Materials R&D problems in Japan



O. Isayev, Nature 2019

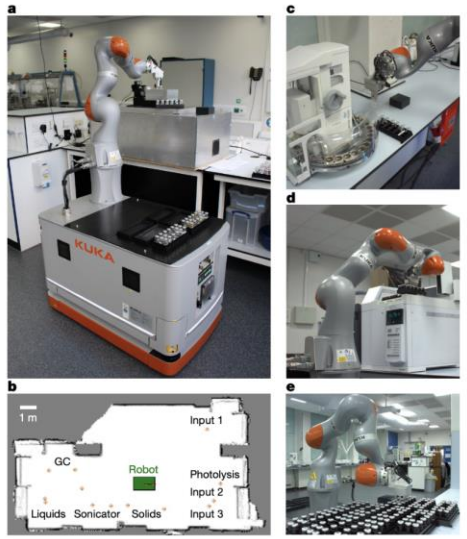
Little materials have been explored on “materials map” (combination : 10^{60}) .
How high-throughput new materials are explored is the key technology.

1. Background

1-2 Materials R&D problems in Japan

Article

A mobile robotic chemist

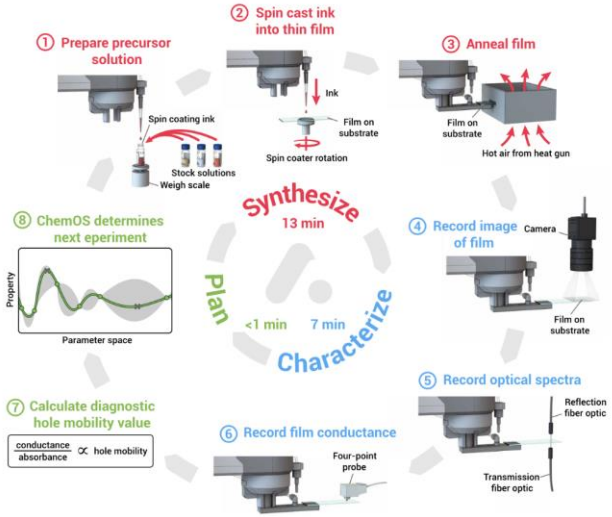


University of Liverpool
Nature 2020

- Catalytic material
- 6 times activity

MATERIALS SCIENCE

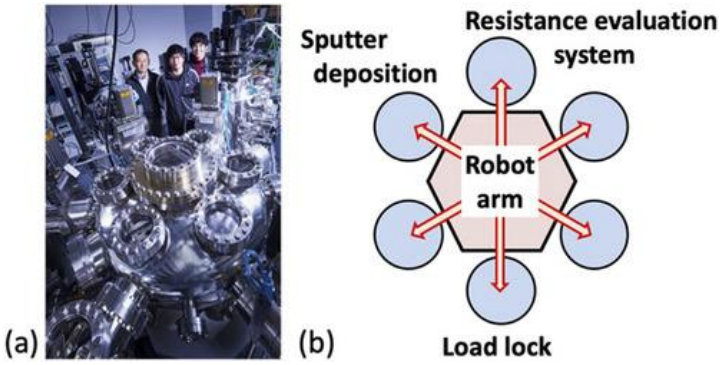
Self-driving laboratory for accelerated discovery of thin-film materials



University of British Columbia
Sci. Adv. 2020

- Organic material
- 9 moths → 5 days

Autonomous materials synthesis by machine learning and robotics



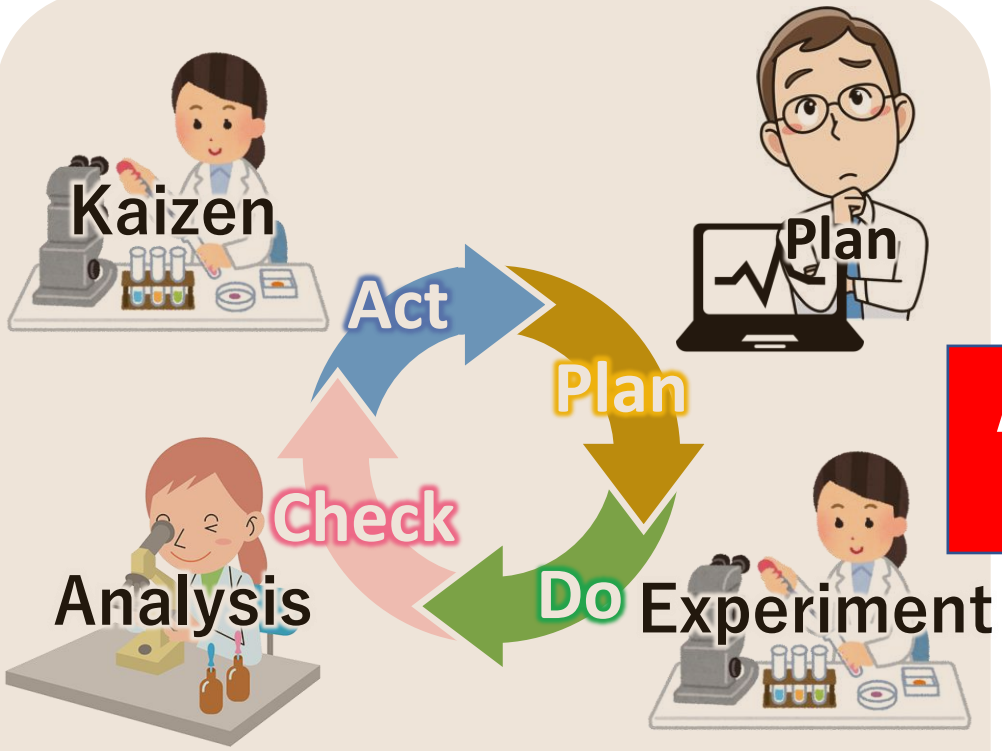
Tokyo Tech.
APL Mater. 2020

- Inorganic material
- 10 times throughput

The use of autonomous exploration tools is drastically advancing in these years.

1. Background

1-2 Materials R&D problems in Japan

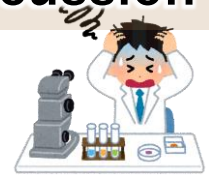


Hypothesis-driven method depending on human

At this rate

①Limited number of trials&errors

②Insufficient discussion



③Repeating same mistakes

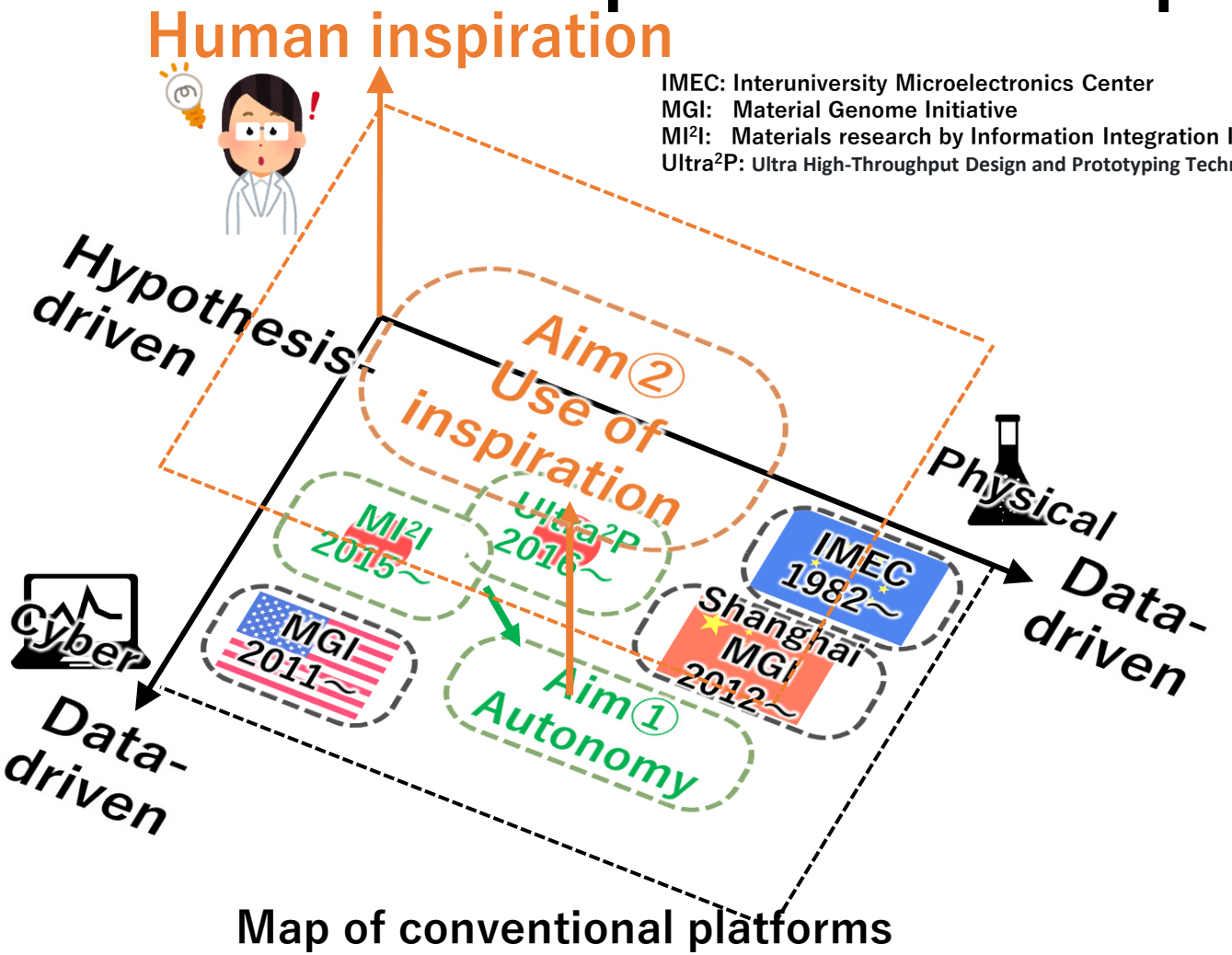
After that

Japan materials industry crisis by low speed research

Materials R&D is Japan “home art”, with rich intuition and experience
However, this hypothesis-driven method will limit “home art”.

1. Background

1-2 Materials R&D problems in Japan



Map of conventional platforms

While each country is working with individual approach, now we need a new platform suitable for Japan

①Autonomy
②Use of inspiration

Outline

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2-2 ①Beyond human activity →HT autonomous systems

2-3 ②Beyond human knowledge→ Data-driven “Hybrid” method

2-4 ③Gather human knowledge → Knowledge sharing

3. Research contents

3-1 Research organization

3-2 Research plan

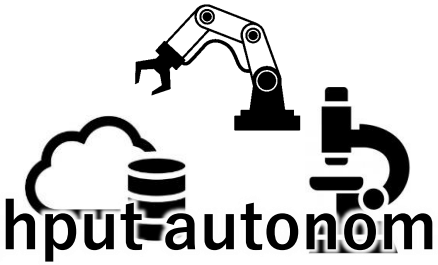
4. Summary

2. Factors and measures

2-1 Extension of materials exploration space

①Limited number of trials&errors

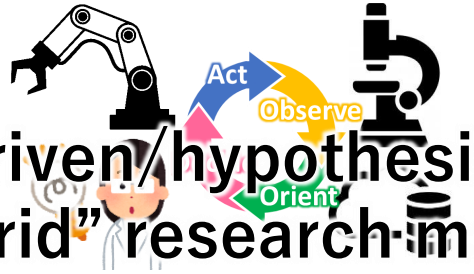
Beyond human activity



High-throughput autonomous systems

②Insufficient discussion

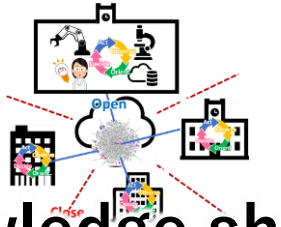
Beyond human knowledge



Data-driven/hypothesis-driven “hybrid” research method

③Repeating same mistakes

Gather human knowledge



Knowledge sharing

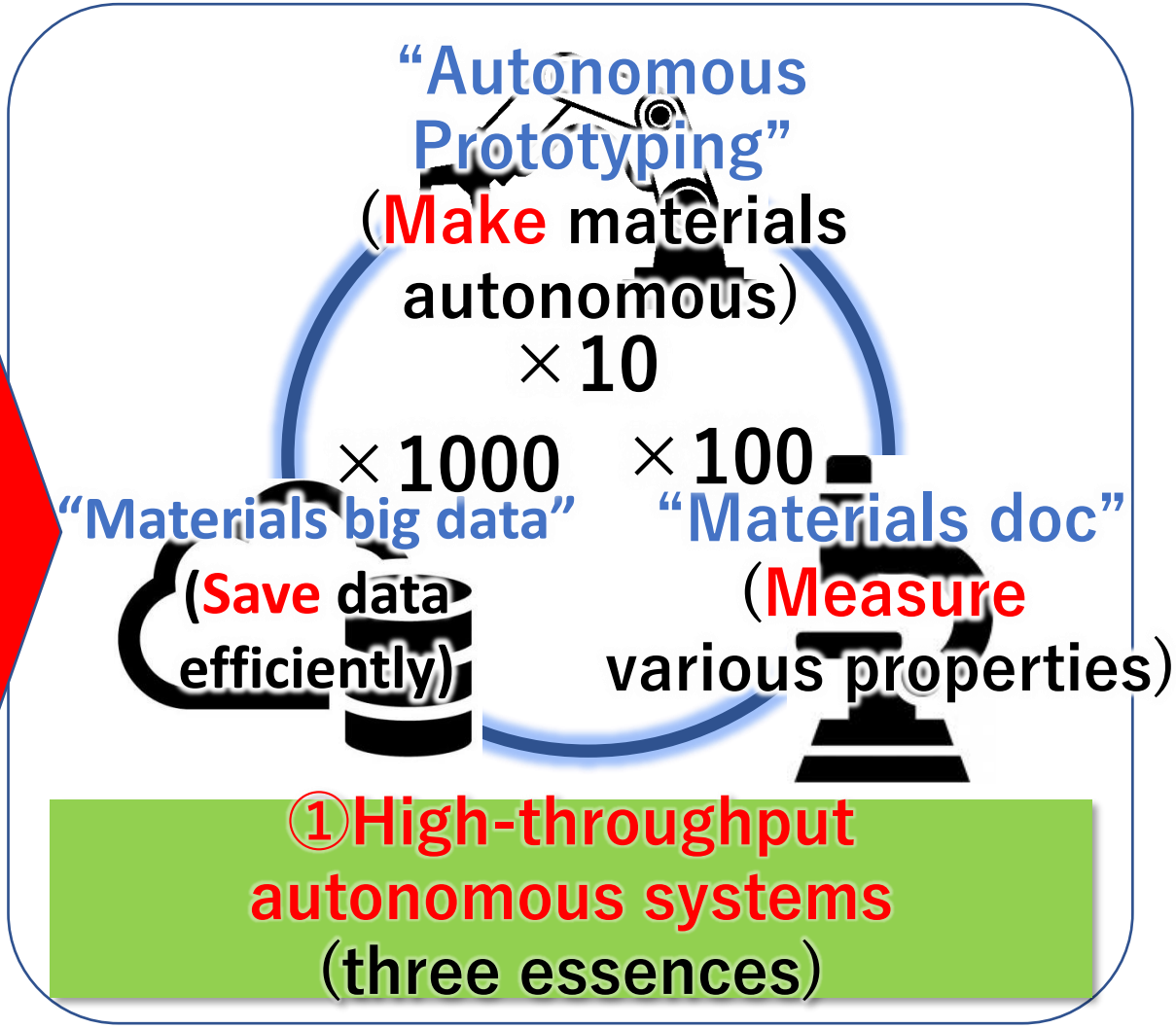
We planned three measures: Our main contents

2. Factors and measures

2-2 ①Beyond human activity →HT autonomous systems

Human-depended works

Beyond human activity

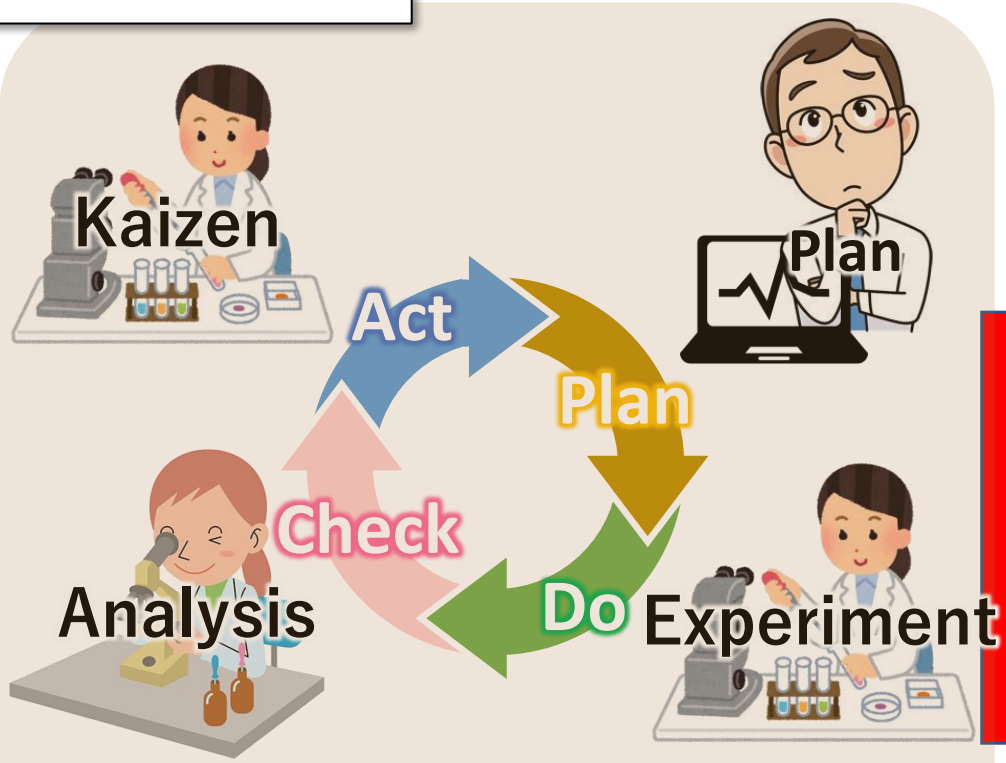


①High-throughput autonomous systems (three essences)

① Element technology for autonomy

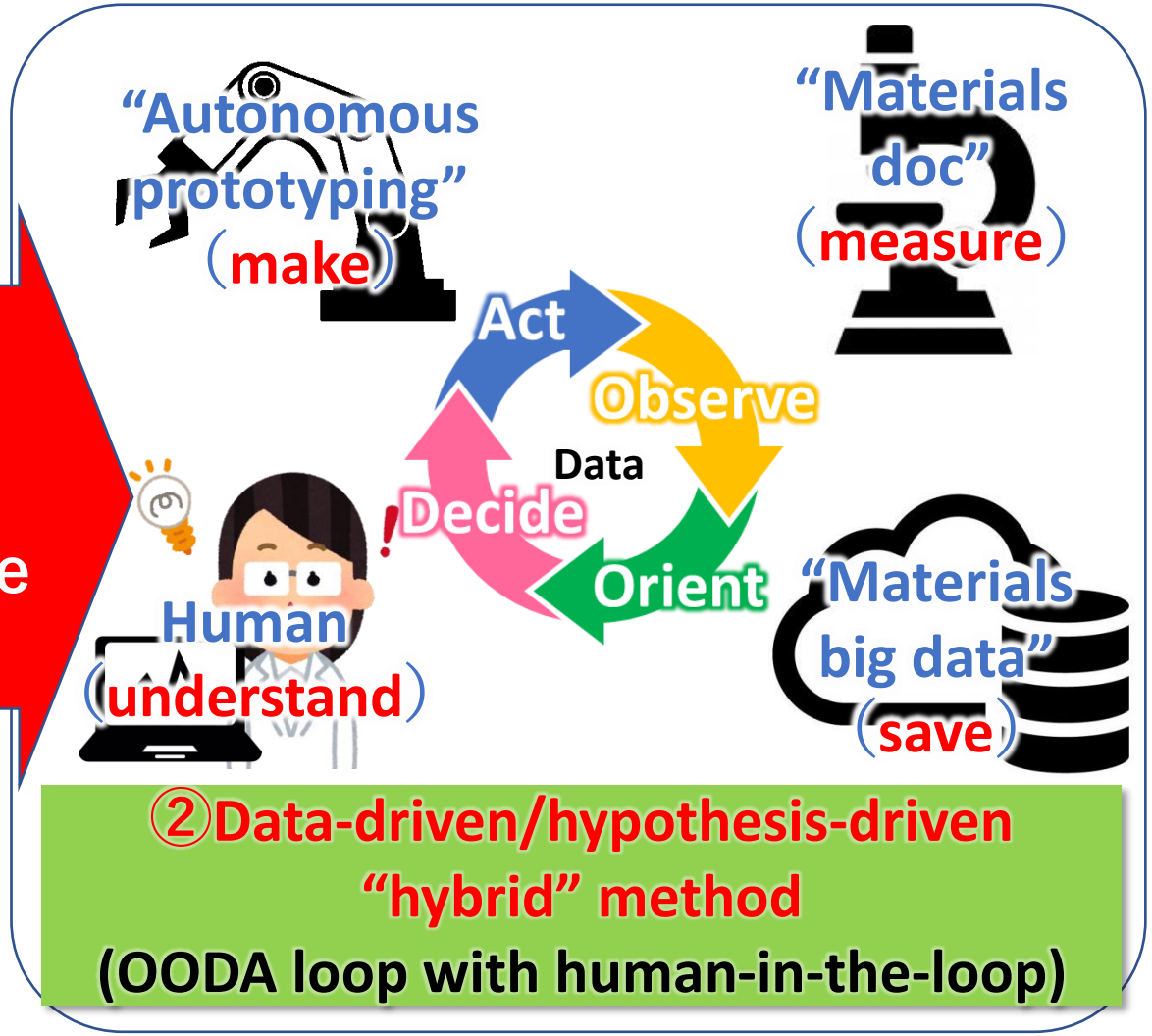
2. Factors and measures

2-3 ②Beyond human knowledge →Data-driven “hybrid” method



Hypothesis-driven method depending on human

Beyond Human knowledge

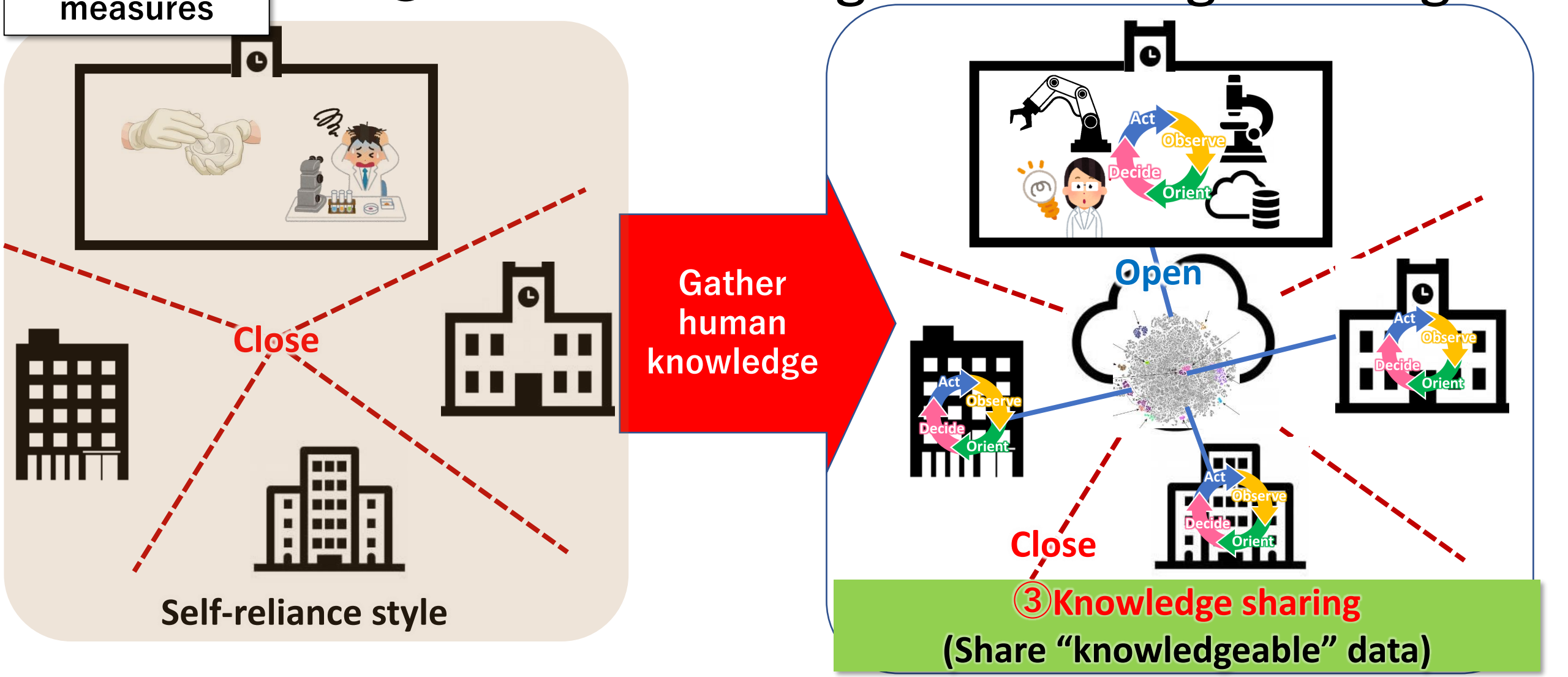


②Data-driven/hypothesis-driven “hybrid” method
(OODA loop with human-in-the-loop)

② Induction and utilization of human inspiration

2. Factors and measures

2-4 ③Gather knowledge →Knowledge sharing



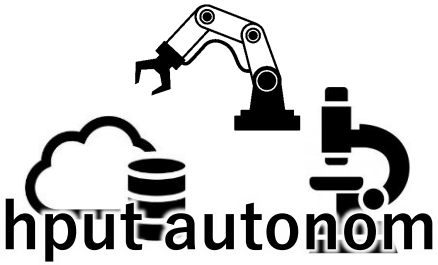
③ Challenge beyond ① “autonomy” & ② “human inspiration”

2. Factors and measures

2-1 Extension of materials exploration space

①Limited number of trials&errors

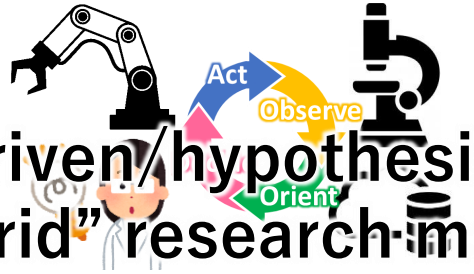
Beyond human activity



High-throughput autonomous systems

②Insufficient discussion

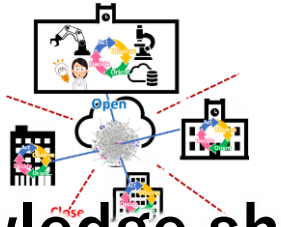
Beyond human knowledge



Data-driven/hypothesis-driven “hybrid” research method

③Repeating same mistakes

Gather human knowledge



Knowledge sharing

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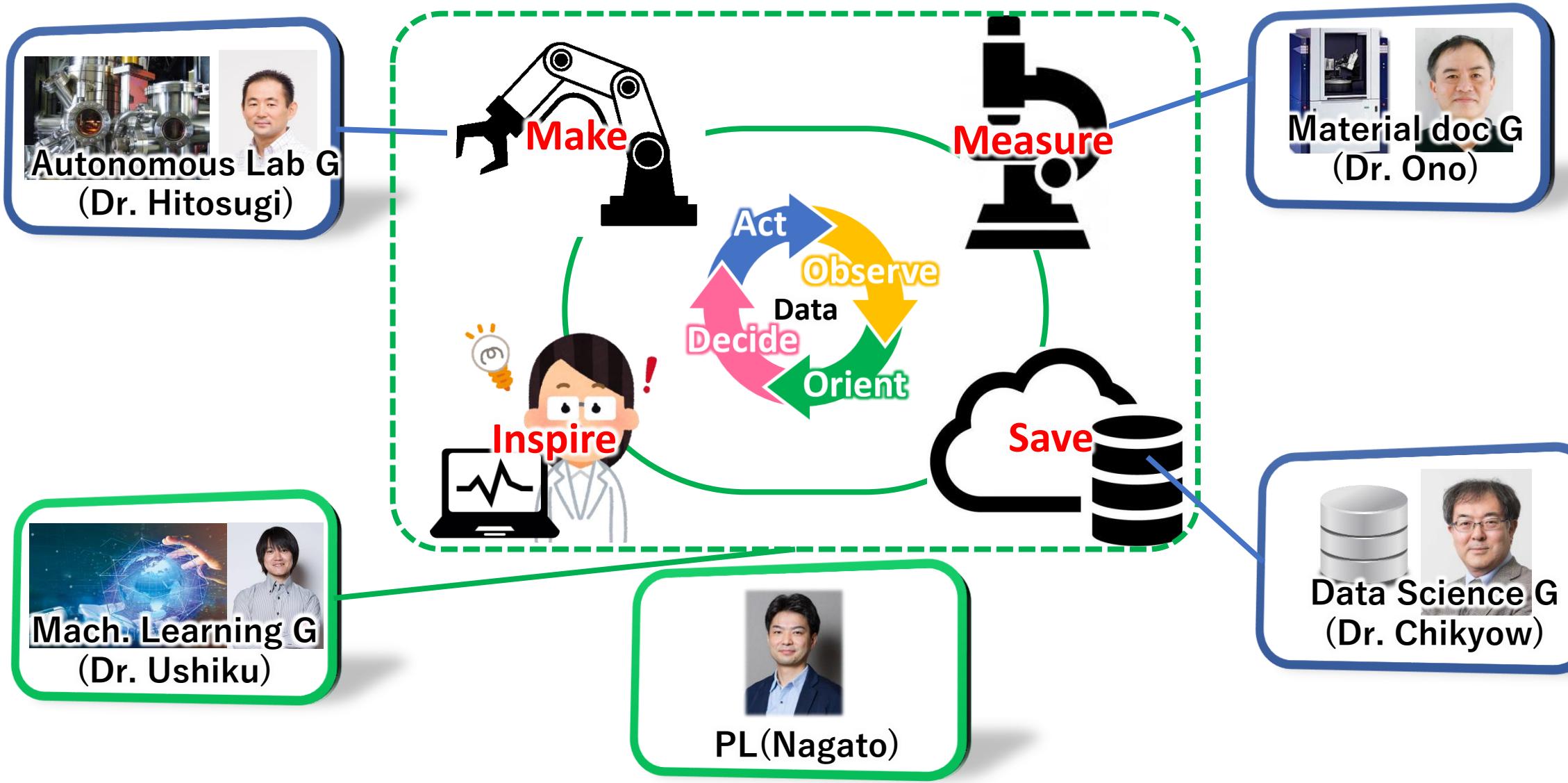
3-2 Research plan

4. Summary

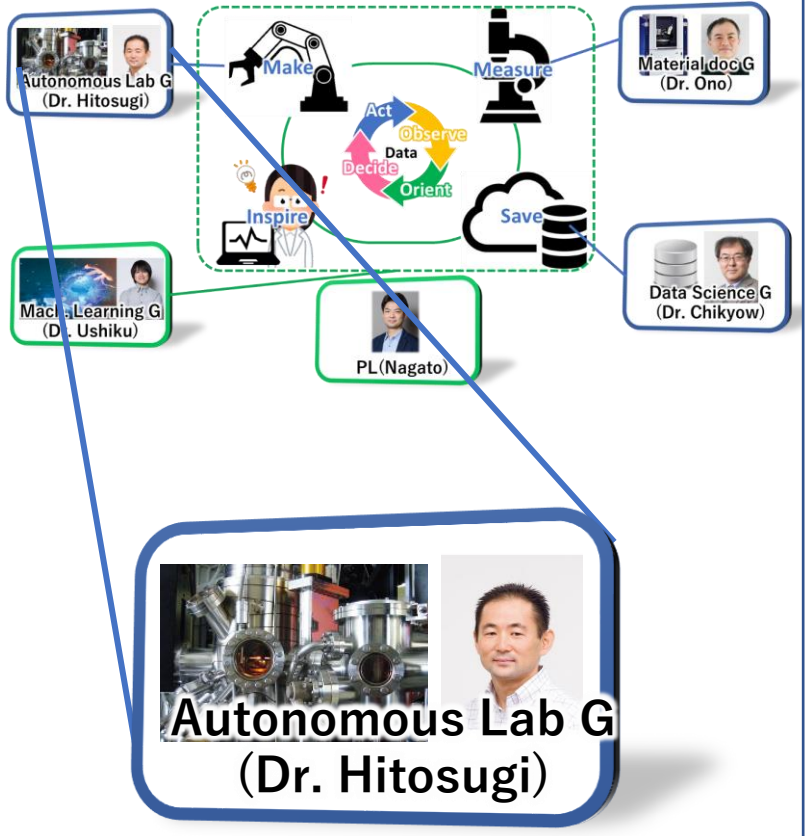
3. Research contents

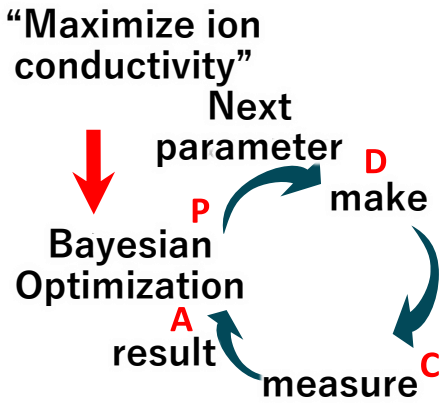
3-1 Research organization

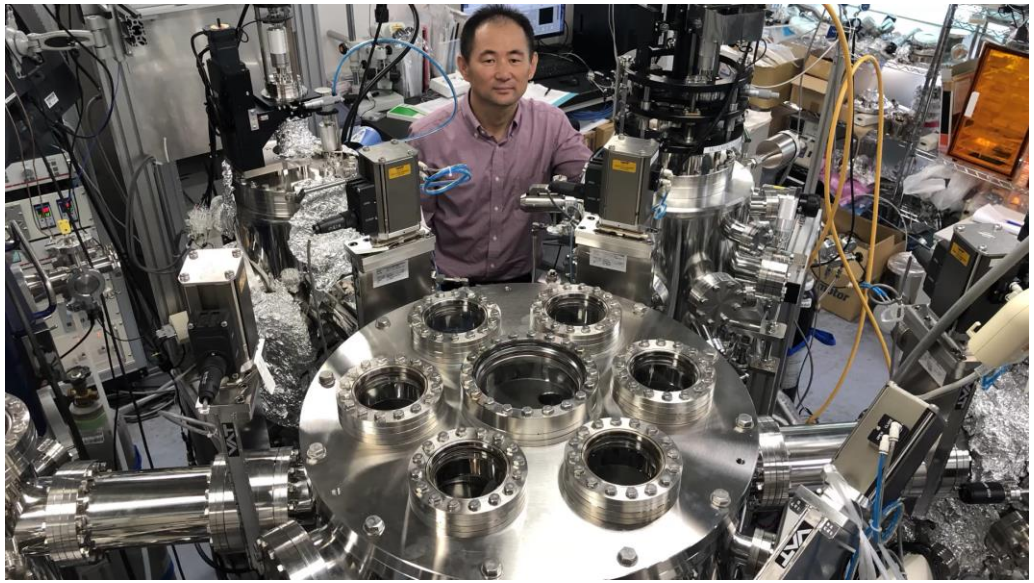


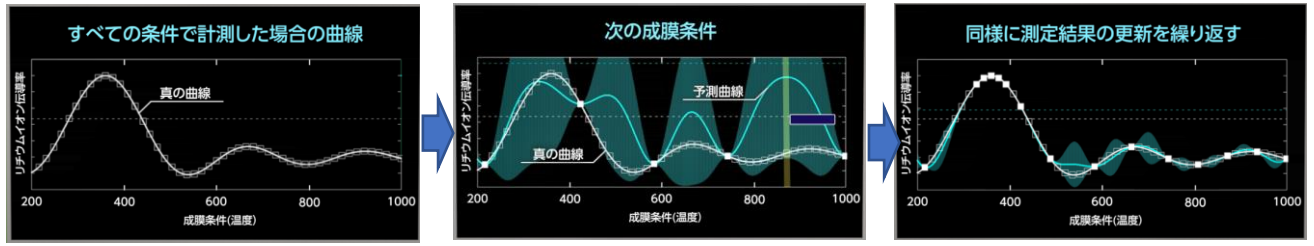
3. Research contents

3-1 Research organization







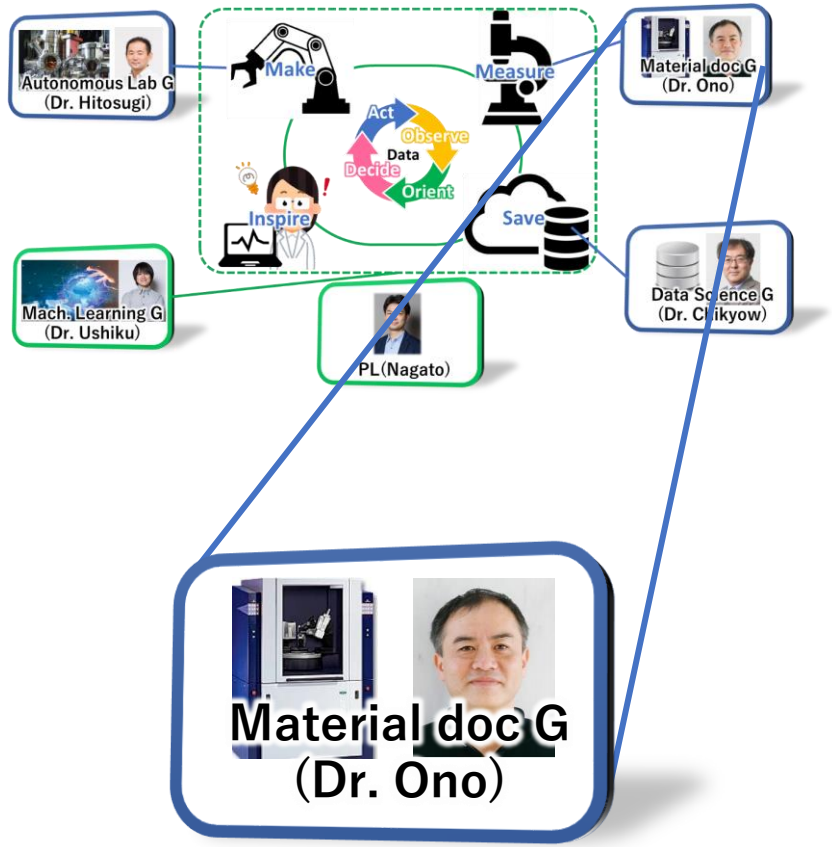


Autonomous exploration of ion-conducting materials with vacuum film formation

Materials are prototyped with autonomous experiment system

3. Research contents

3-1 Research organization

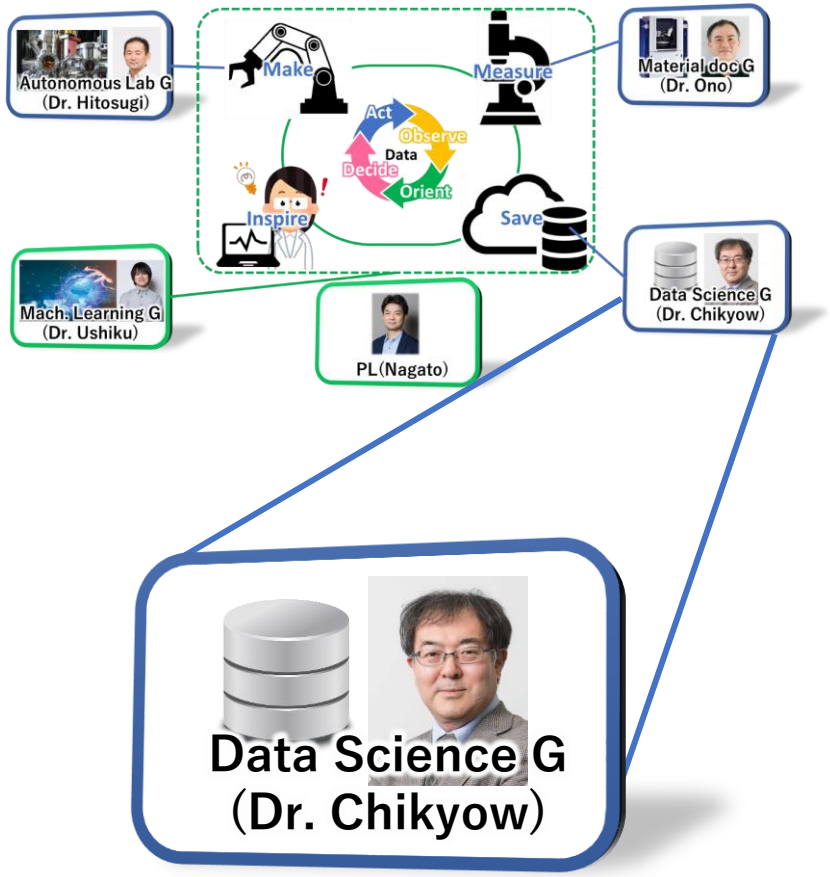


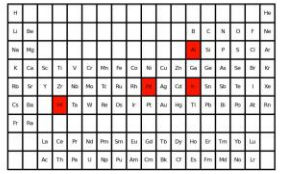
“Materials doc” extracts knowledge from various properties measured by various method

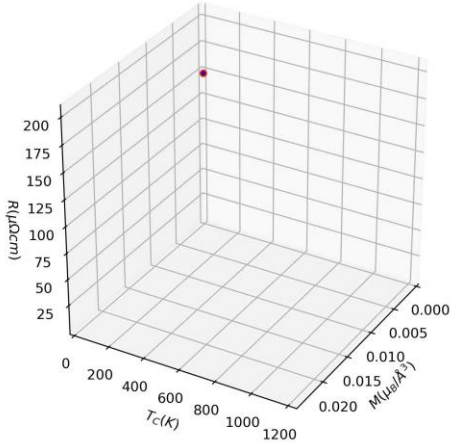
Knowledge is identified from various measurement.

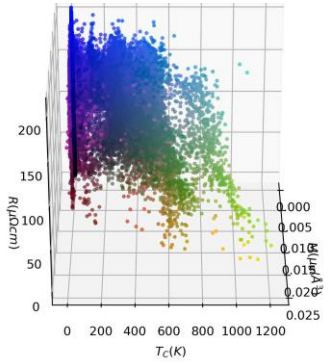
3. Research contents

3-1 Research organization

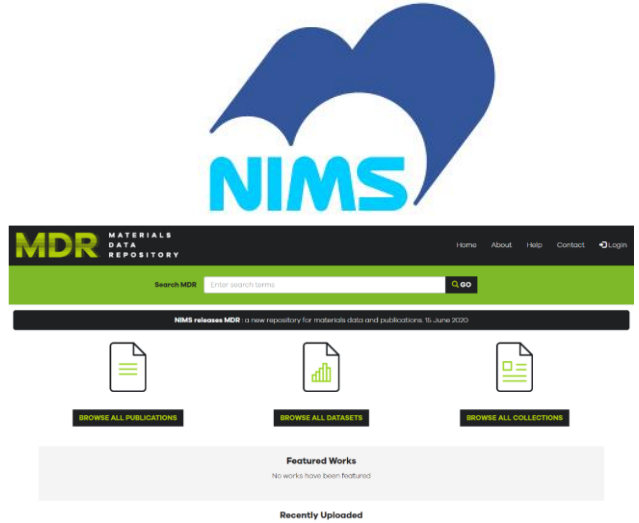








Prediction of new materials in cyber space

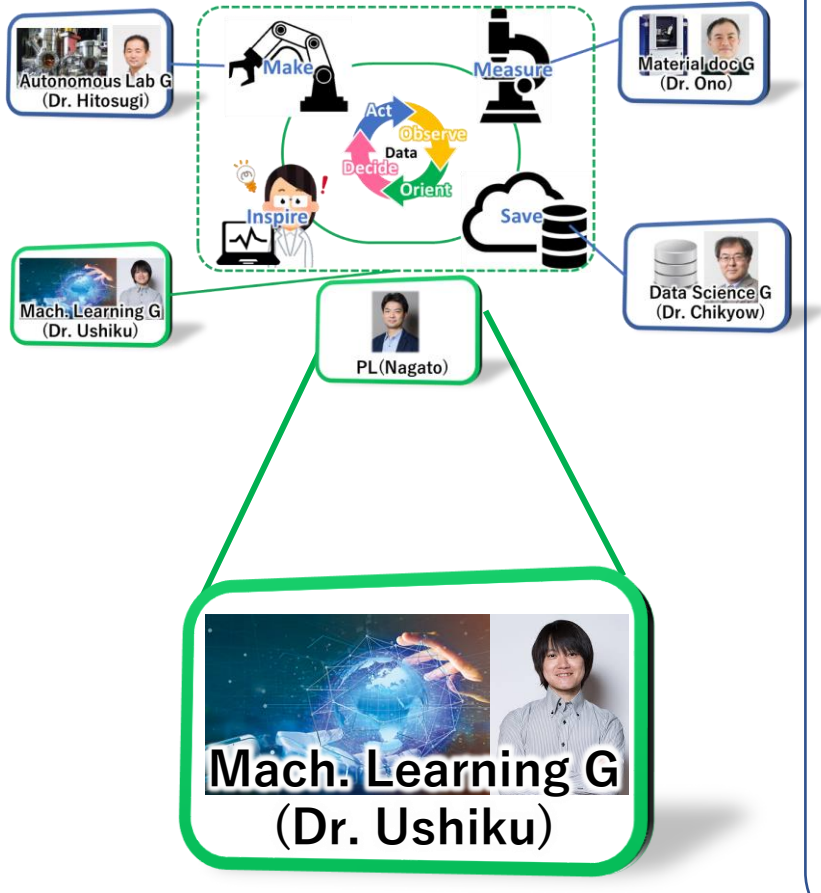


Early adapting NIMS data platform center

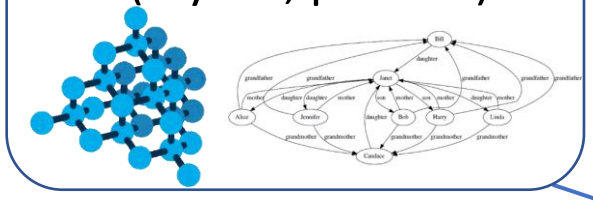
Next candidate is predicted from identified knowledge

3. Research contents

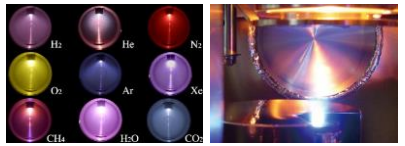
3-1 Research organization



Graph
(crystal, process)



Sequence
(image, video)

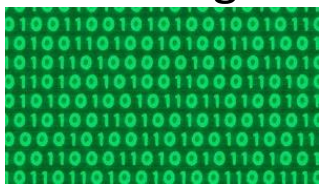


Series
(sensor, language)

Correlation

Cause and Effect

Symbolic regression



$$y = \frac{mg}{k}t - \frac{m^2}{k^2}$$

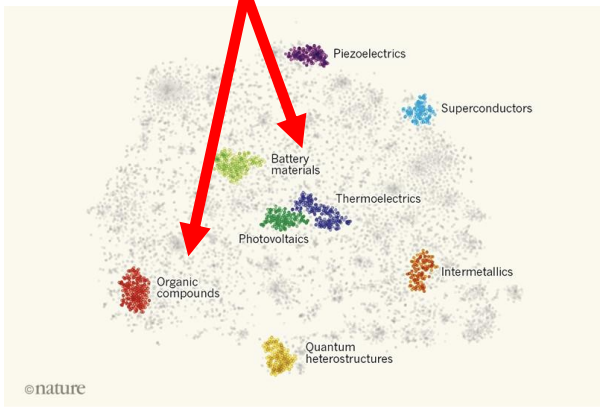
Explainable machine learning (AI)
→Transit tacit knowledge
to explicit knowledge

Cleansing of data to trigger human inspiring.

3. Research contents

3-2 Research contents

Gray: not yet explored

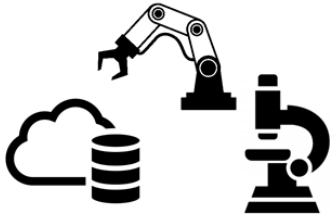


O. Isayev, Nature 2019

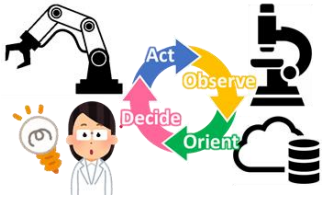
Ambitious part: not yet explored

a colored version of the map of the once known world from Martin Waldseemüller, 1507

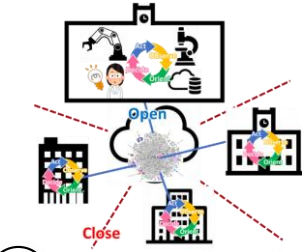
“Age of Materials Discovery” （※ named by our group）



①High-throughput Autonomous system ＝ **High-speed boat**



②Data-/hypothesis-driven Hybrid method ＝ **Compass**

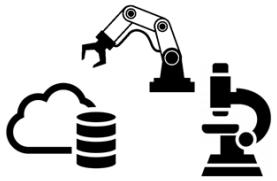
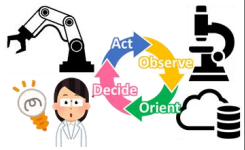
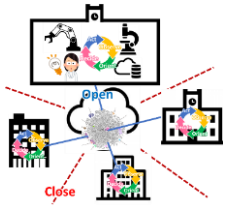


③Knowledge sharing ＝ **Navigation act**

Our POC extends materials exploration space with these three measures

3. Research contents

3-2 Research contents

Contents		2021	2022	2023	2024	2025
①High-throughput Autonomous systems 	High-speed boat 	Autonomous lab(AL) Design/launch				
		Mater. Doc (MI) Element technol.				
②Data-driven Hybrid method 	Compass 	Prediction of new materials with MI		Demo. Human-in-the-loop	Demonstration of exploration of battery materials ・All solid-state battery material ・Throughput: 1,000 times	
		Develop data cleansing method				
③Knowledge sharing 	Navigation act 		Trial of AL from outside institute			
		Data sharing infrastructure Design/launch				

Step1: Development of element technology for ①② HT systems

Step2: Demonstration of ③Knowledge sharing

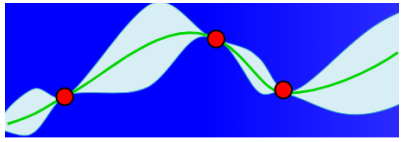
Step3: High-throughput development of battery materials KPI: 1,000 times

3. Research contents

3-2 Research contents

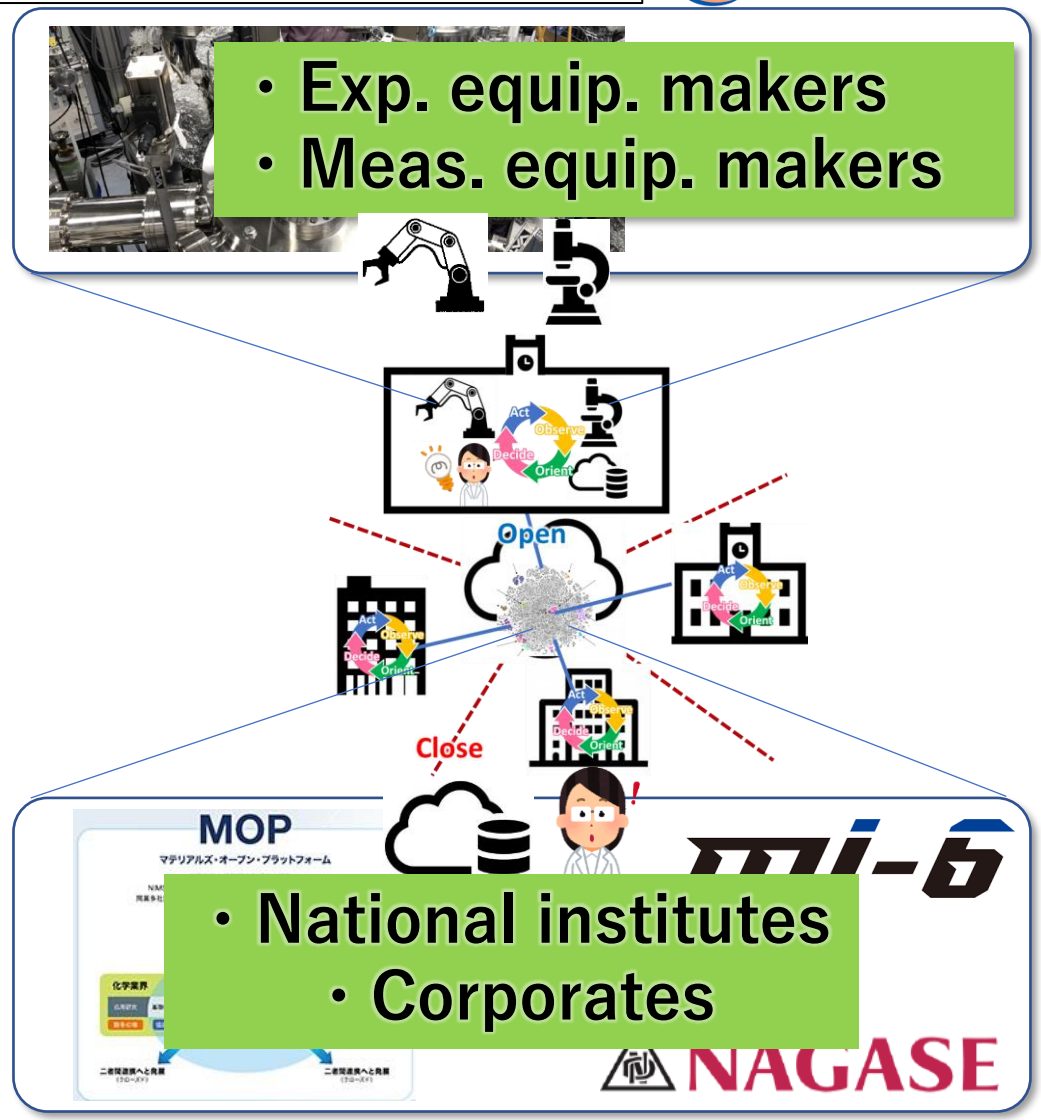
Students：62(2020)

Collaborative Education ：24



公益社団法人 応用物理学会 Japan Society of Applied Physics

Informatics application research group: 23



We aim platform of human-resource and industry/academia collaboration

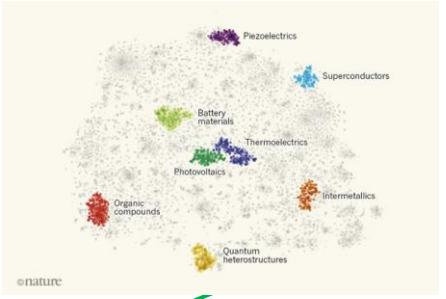
We aim ecosystem of materials exploration

Outline

1. Background

1-1 Social Issues surrounding Materials R&D

1-2 Materials R&D problems in Japan



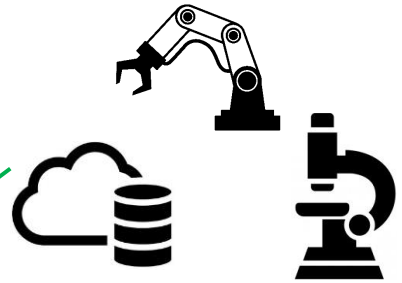
2. Factors and Measures

2-1 Extension of materials exploration space

2-2 ①Beyond human activity →HT autonomous systems

2-3 ②Beyond human knowledge→ Data-driven “Hybrid” method

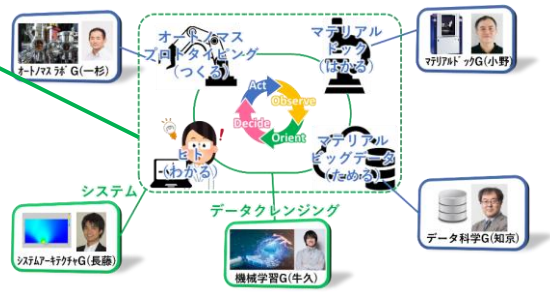
2-4 ③Gather human knowledge → Knowledge sharing

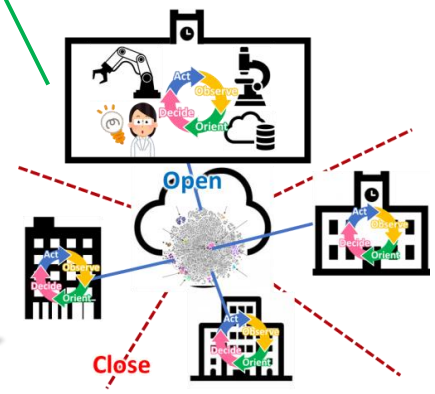


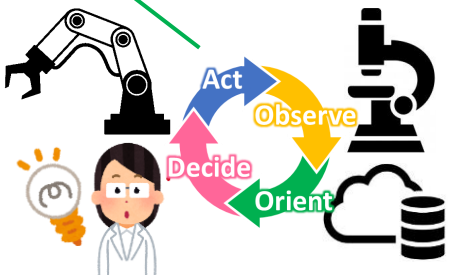
3. Research contents

3-1 Research organization

3-2 Research plan







4. Summary

4. Summary

MEEP

Materials Exploration space Extension Platform

We are small-starting in Japan.
But we need international collaboration.
Please contact us and welcome our contacting.

4. Summary

MEEP

Materials Exploration space Extension Platform

Departure ‘Age of Materials Discovery’ together!

Thank you for your attention.