MaDIS
NIMS MATERIALS DATA and INTEGRATED SYSTEM

National Institute for Material Science

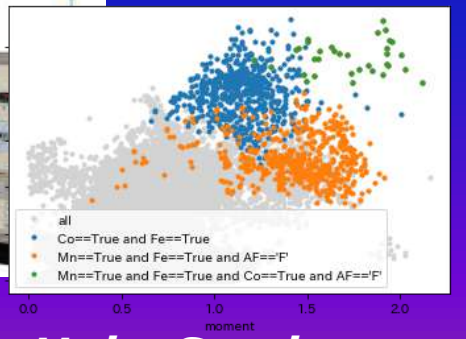
NIMS

実験家からみた
マテリアルズインフォマティクスと今後の展望

Impact of Materials Informatics for Experimentalists and future vision of Materials Research

Toyohiro Chikyow,
Associate General Director,

NIMS
Materials Data & Integrated System (MaDiS)



2020.5.28 Tohoku Univ. Seminor
東北大学知のフォーラム セミナー

contents

MaDIS
NIMS MATERIALS DATA and INTEGRATED SYSTEM

- Impact of Materials Informatics
- Present status of “Materials Informatics”
- What comes after MI
- Materials Research in future
- Conclusion

Innovation in materials research : AI can discover new materials?

日本経済新聞　2019年(平成31年)2月17日(日曜日)　サイエンス 30

材料開発にAI革命

金属など「職人技」より効率的

マテリアルズ・インフォマティクス　情報科学駆使し探索

材料・製造技術／生活科学

データ分析 多彩な手法

研究開発 AIで進化

開発期間を短縮

80億通りから最適解

赤外線吸収材料 探索2%で開発

混沌を解析

画像認識からデータ化

多層材料からナノシート 少ないデータでも解析

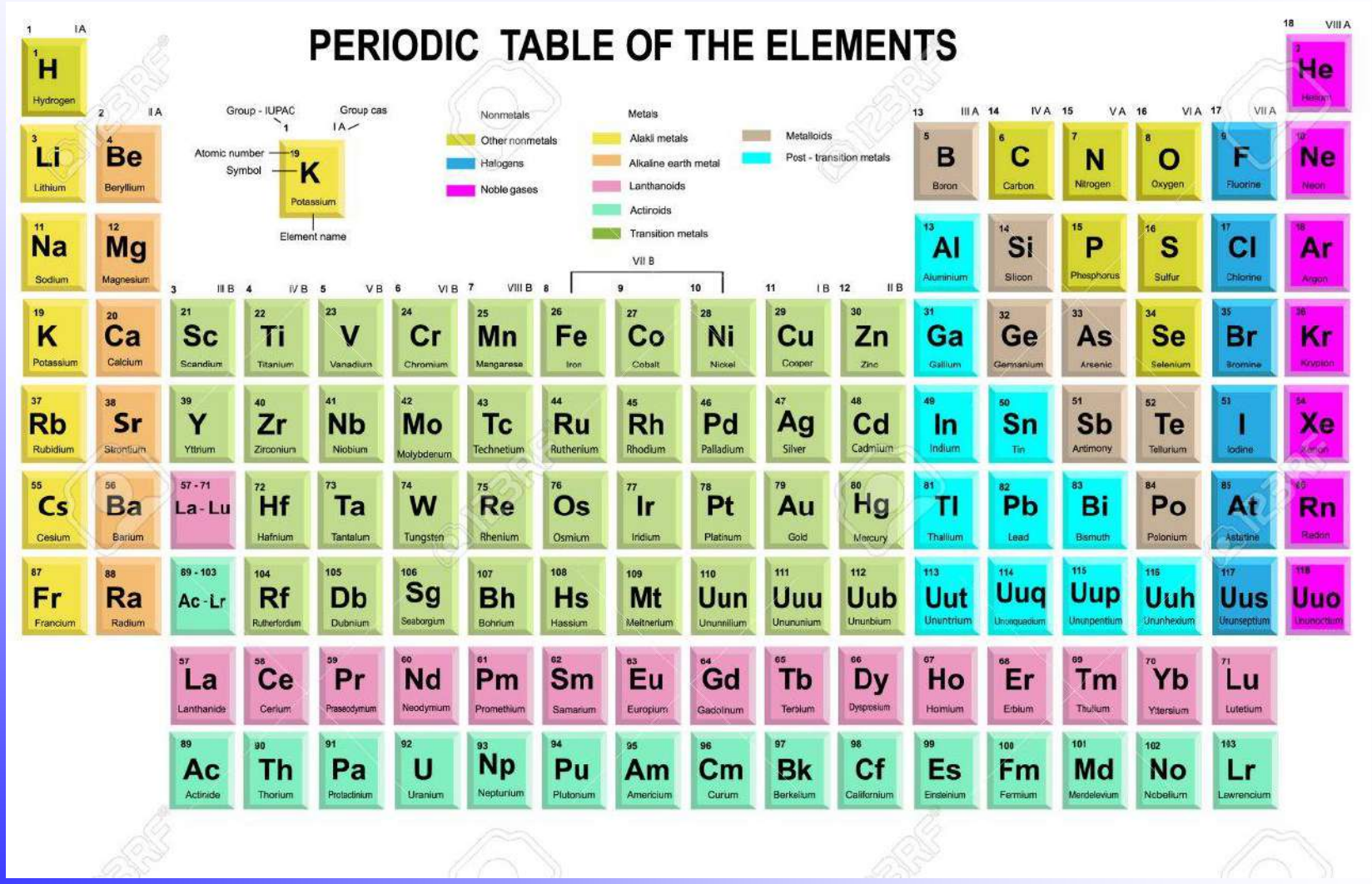
理現象の理解進む

深層断面 SPECIAL EDITION

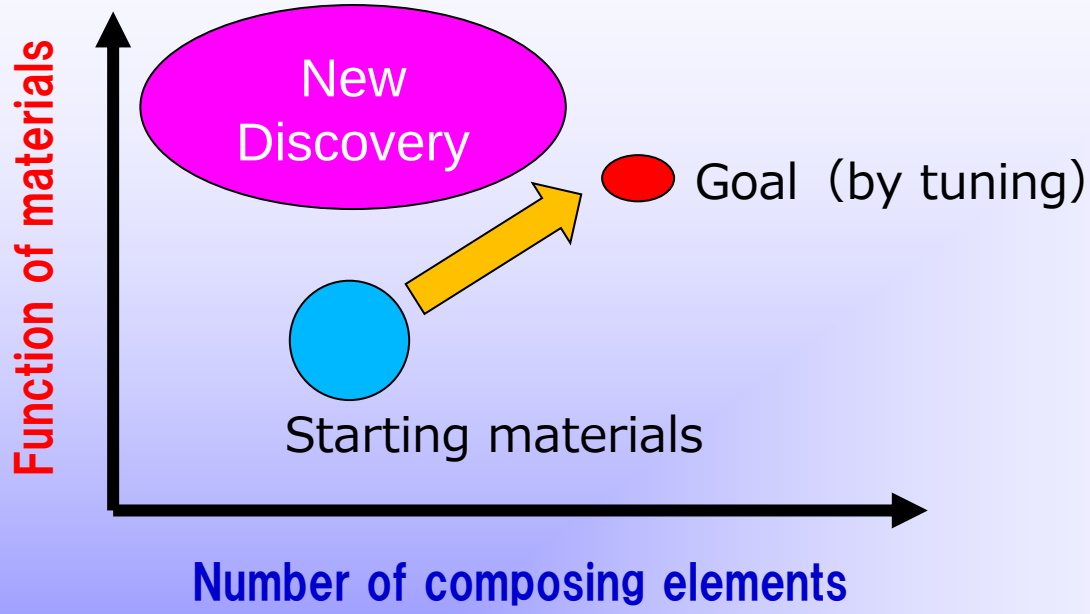
2019年2月17日　日経新聞
Nikkei　Feb.17, 2019

2019年2月1日　日刊工業新聞
Nikkan Indust.news Feb.1 2019

A large variety of the composition in materials



Why new discovery is difficult in materials

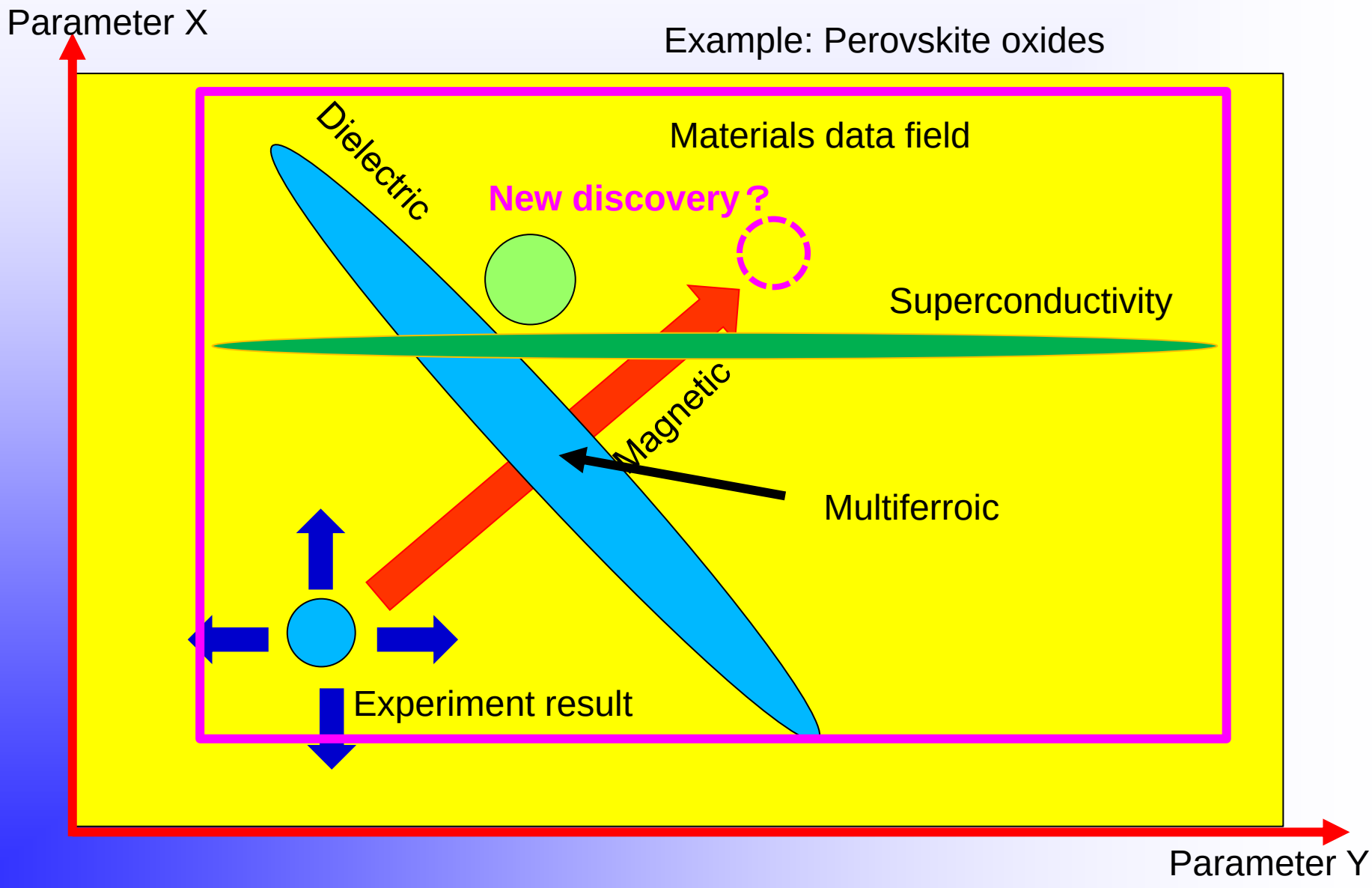


Staring
Basic elements
→ Basic+A
A:impovement
Disadvantage
→ Basic+A+B
A:Improvement
B:Improvement
disadvantage
→ Basic+A+B+C
A:Improvement
B:Improvement
disadvantage
C:Improvement

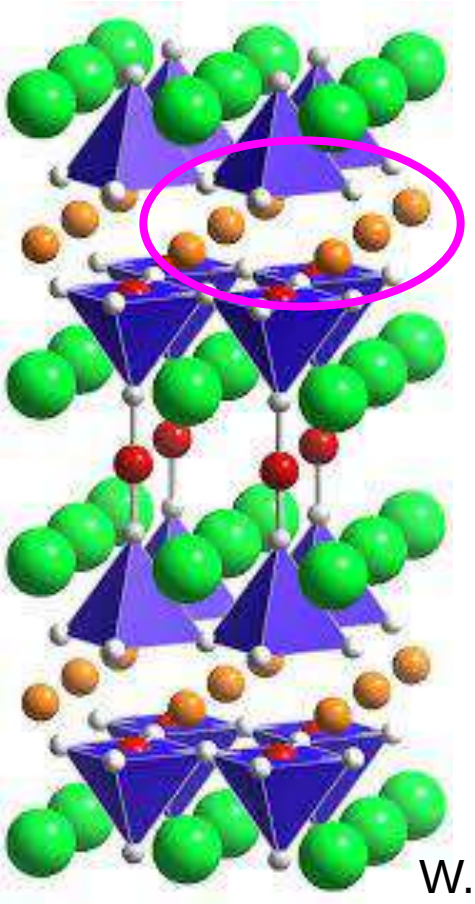
A>B>C

How the experts think in materials design.

National Institute for Material Science

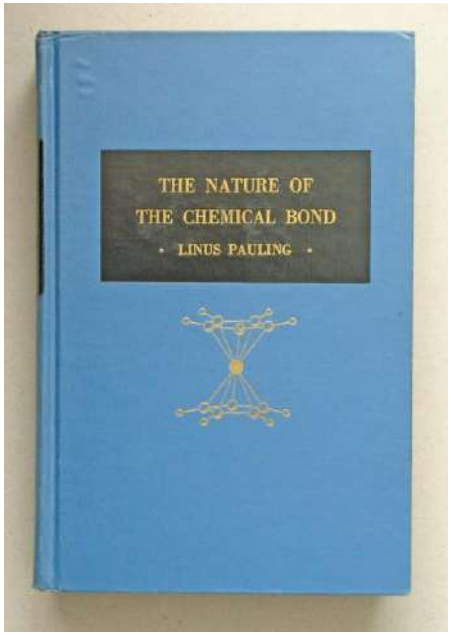


Focusing critical structures and bonds



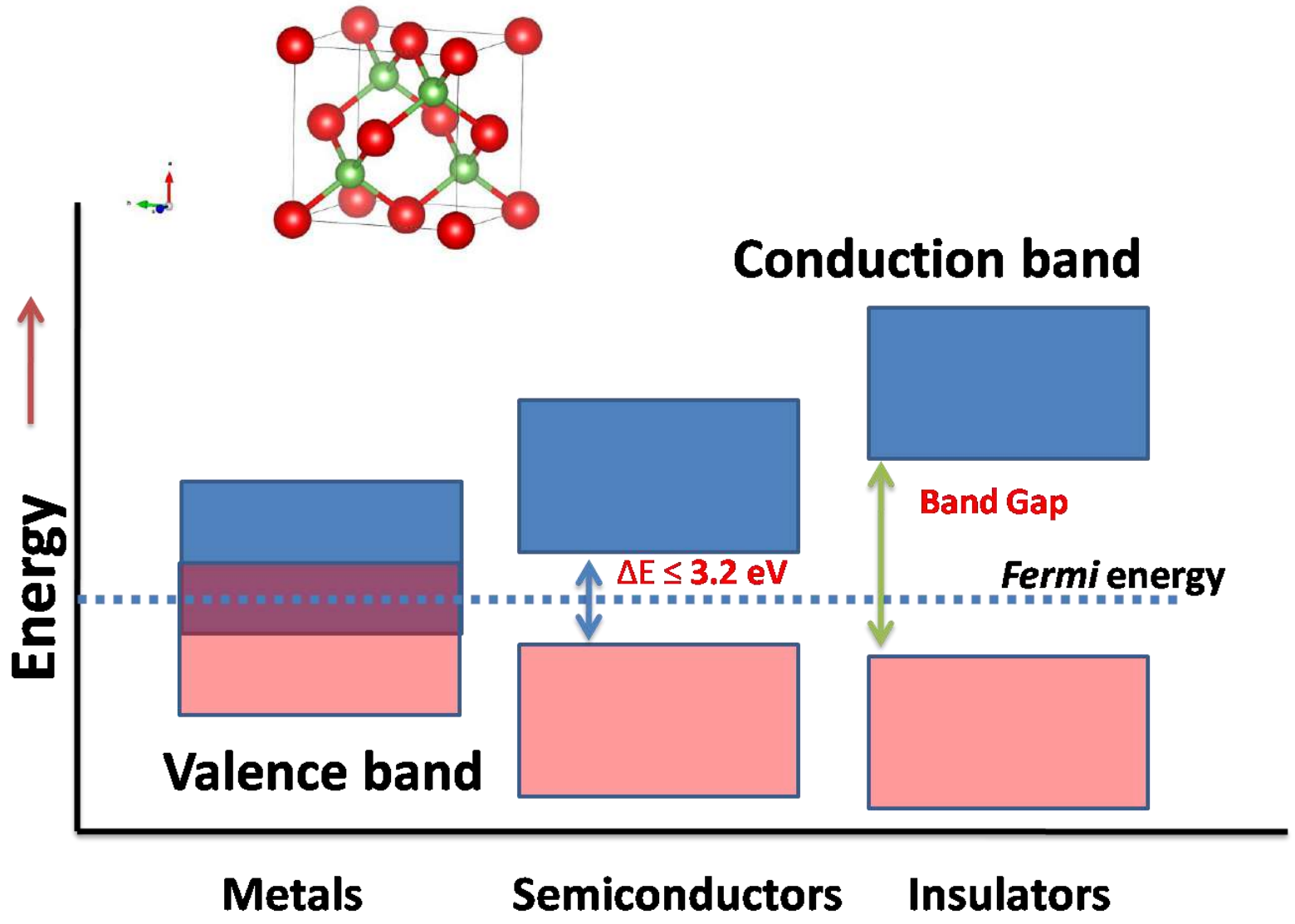
Perovskite Oxides

W.A Harrison：固体の電子構造と物性
Electronic Structure and
the Properties of Solids
=> band gap

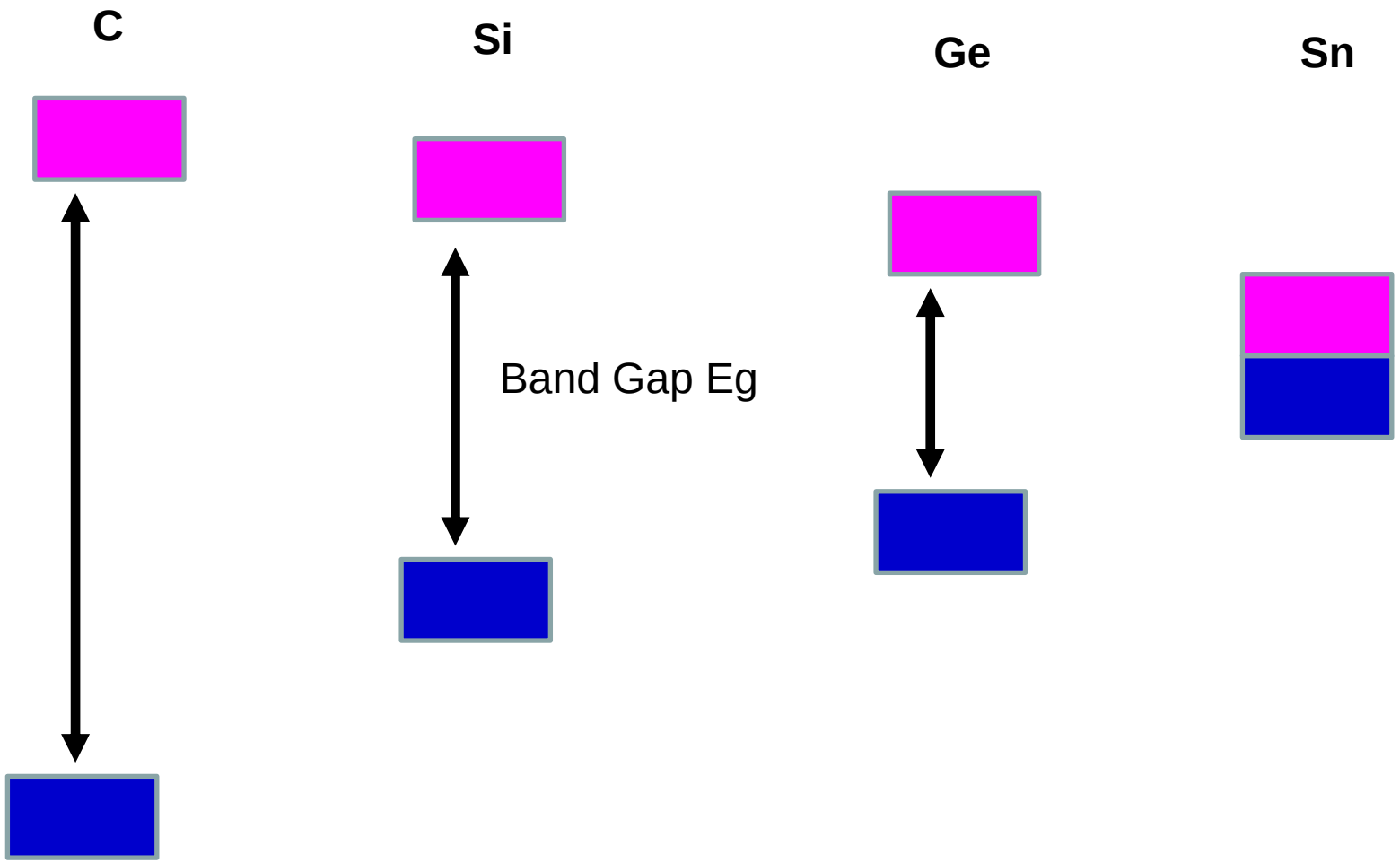


L.Pauling：化学結合論
Nature of chemical Bond
electro negativity
=> Heat of formation

Band Gap


Conduction band
Band Gap
ΔE ≤ 3.2 eV
Fermi energy
Energy
Valence band
Metals
Semiconductors
Insulators

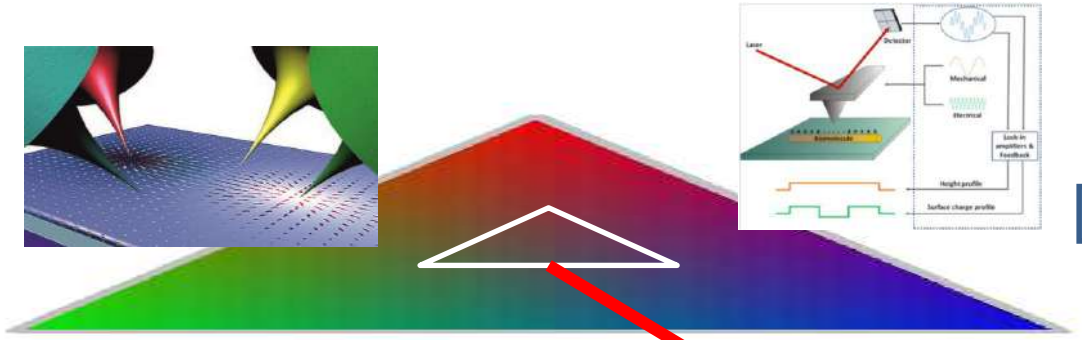
Electric Structure of Semiconductor : IV elements



How we can extend " Materials Data Field" : Challenge for High Throughput experimentation

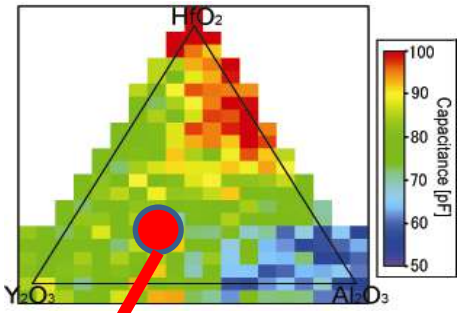
First Screening
（Wide range）

各種走査型
プローブ顕微鏡



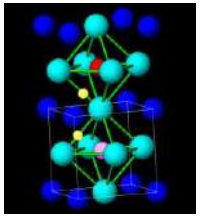
First Screening Time and Cost

Second Screening
（Narrow range)



1) Calc.
2) Simulation
3) Data Science

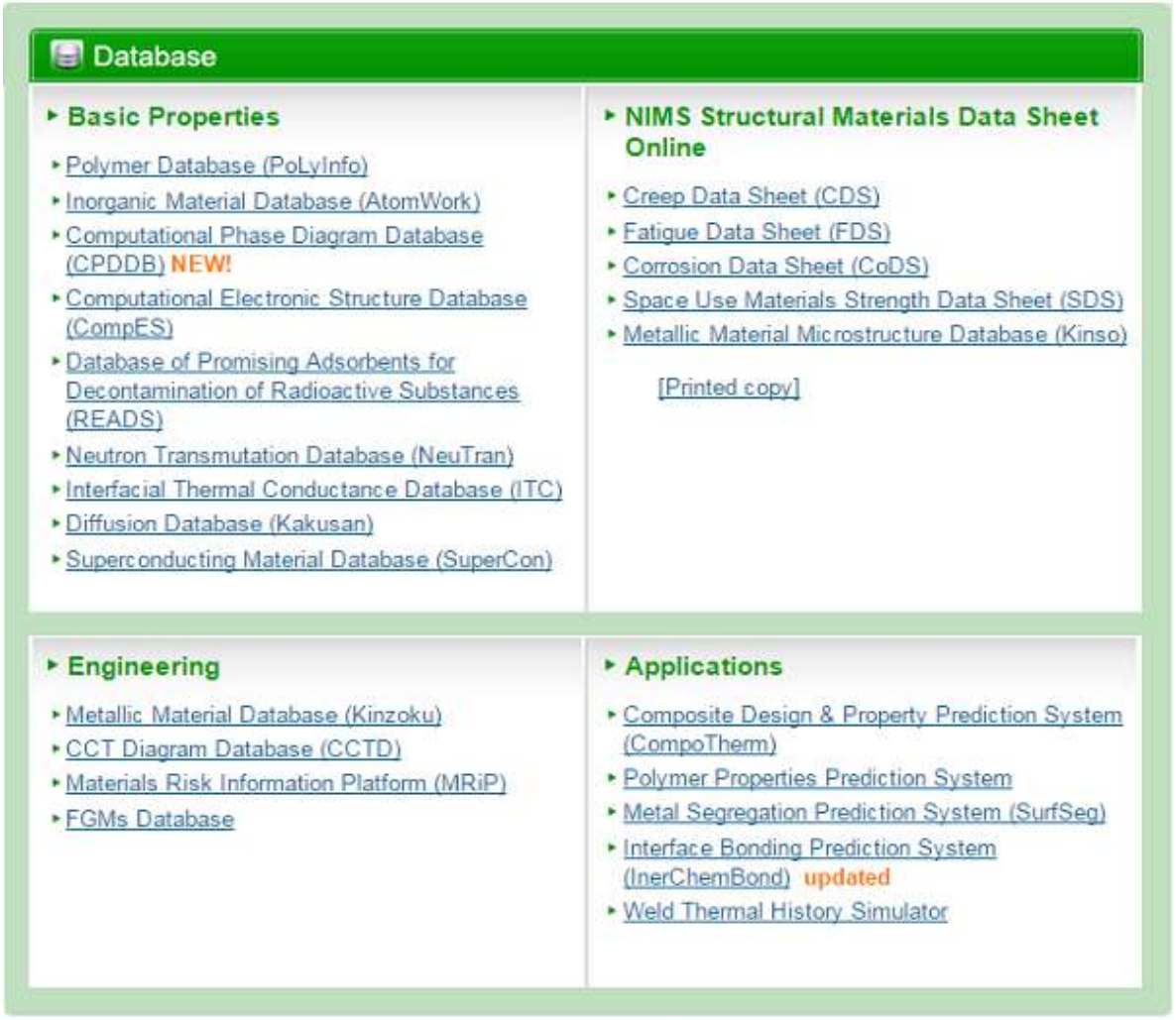
New Materials
Discovery



National project on materials informatics
"Materials Research by Information Integration" Initiative (MI^{2}I)

Mi^{2}i

"MatNavi" is one of the world's largest materials databases provided by NIMS



See the web site,
http://mits.nims.go.jp/index_en.html

"MatNavi" consists of ～20 database (polymer, inorganic materials, superconductivity, etc.) with high reliability.

"MatNavi" provides data visualization tools and simple prediction simulator of material properties.

New materials discovery by “ Computation”

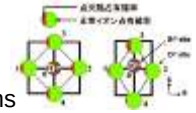
Points: Materials are reviewed by “ Lattice and elements”

NIMS is involved in“Phase” development

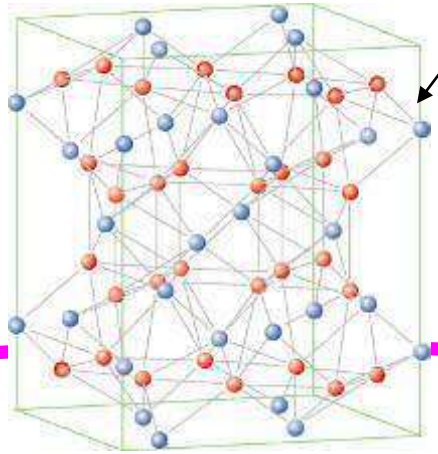
Doping

Plasma doping
by Ishigaki, nims

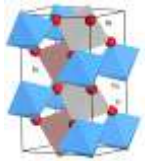
defect



Piezoelectric
by Ren, nims

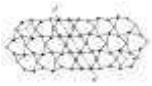


Atomic
arrangement



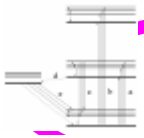
Catalysis
by Ye, nims

Lattice
disorder

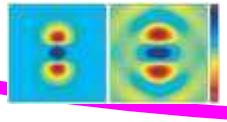


SuperLattice

Single, poly amorphous

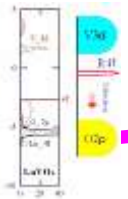


exisiton

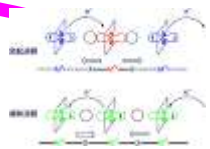


orbital

Spin



bandgap

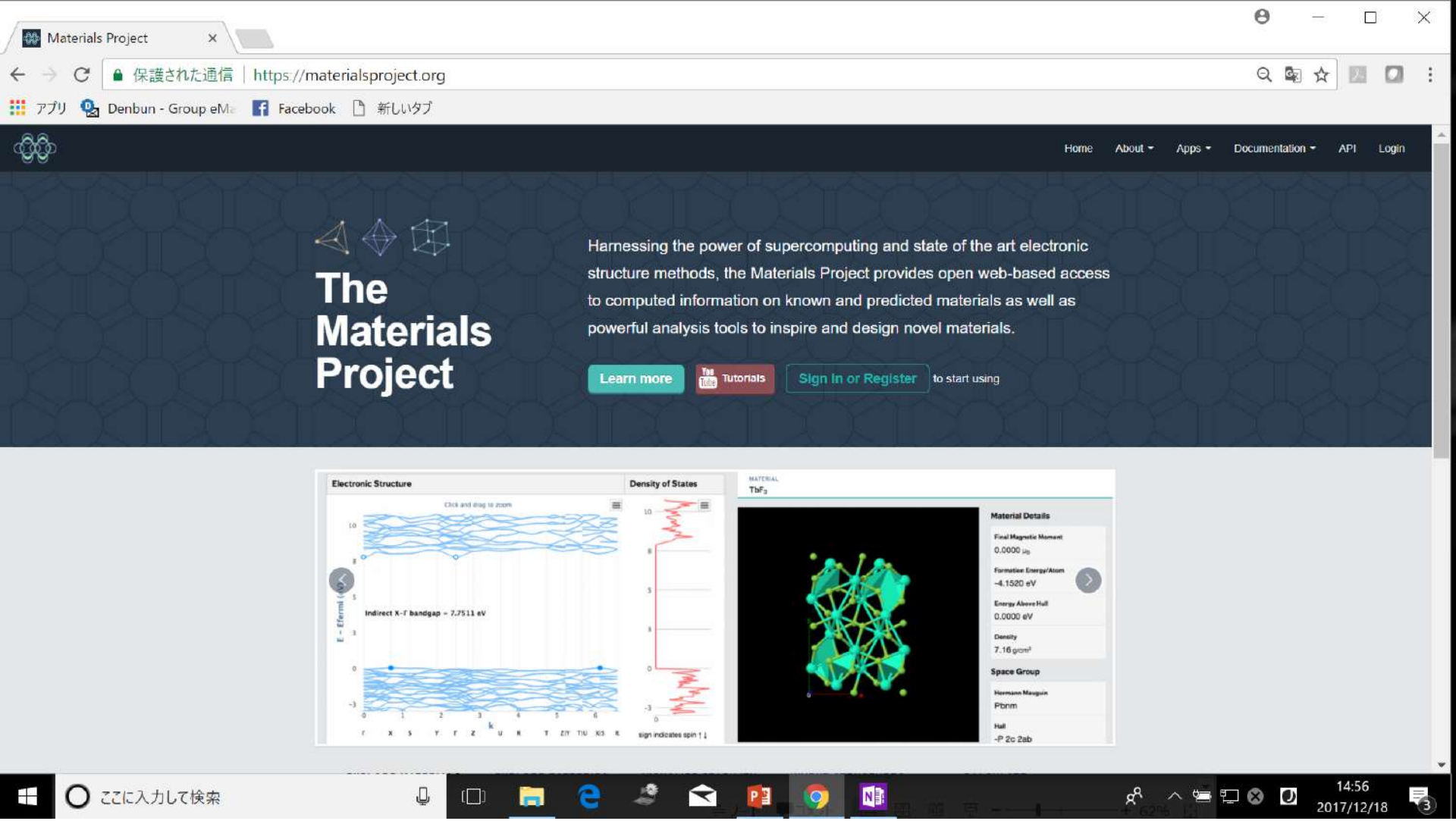


phonon

dielectric strength magnetization Thermolectric density

piezoelectric luminescence conductivity Light emission Photonics Thermal conductivity

Design new materials which does not exist before

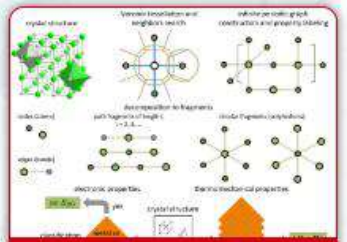


Prof. Gerbrand Ceder
(Professor, UC Berkeley)

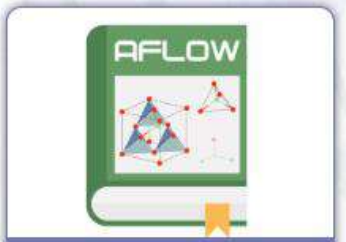
https://materialsproject.org/

Apps and Docs

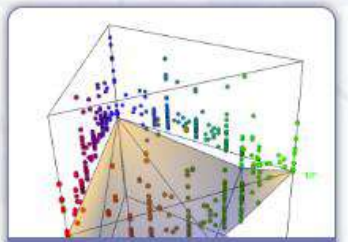
MendeLIB search



AFLOW-ML

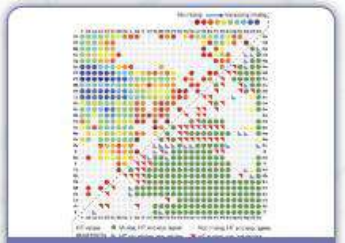


Crystal prototypes

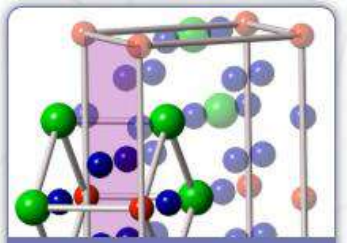


AFLOW CHULL

Aflow-online



Binary alloy library



Superalloys search

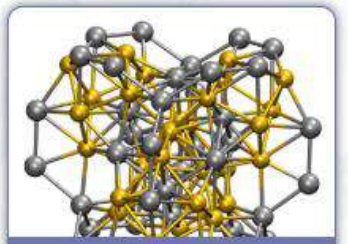
AFLOW
REST-API WIKI

Documentation

AFLOWπ

PAOFLOW

Geolocation data



Showcase material

Duke UNIVERSITY

ONR Science & Technology

U.S. DEPARTMENT OF ENERGY

NSF

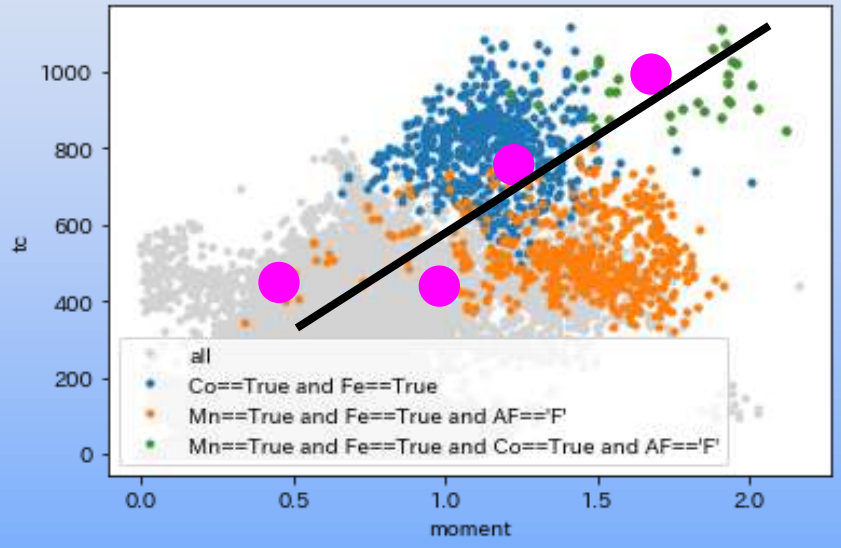
Homeland Security

CRAY THE SUPERCOMPUTER COMPANY

UNT

Automatic Work Flow from database to calculation

- **Automatic flow to select parameters in DFT Calculation and Energy integration region**
- **Demonstration of quaternary high entropy alloy automatic calculation for magnetic alloy survey**



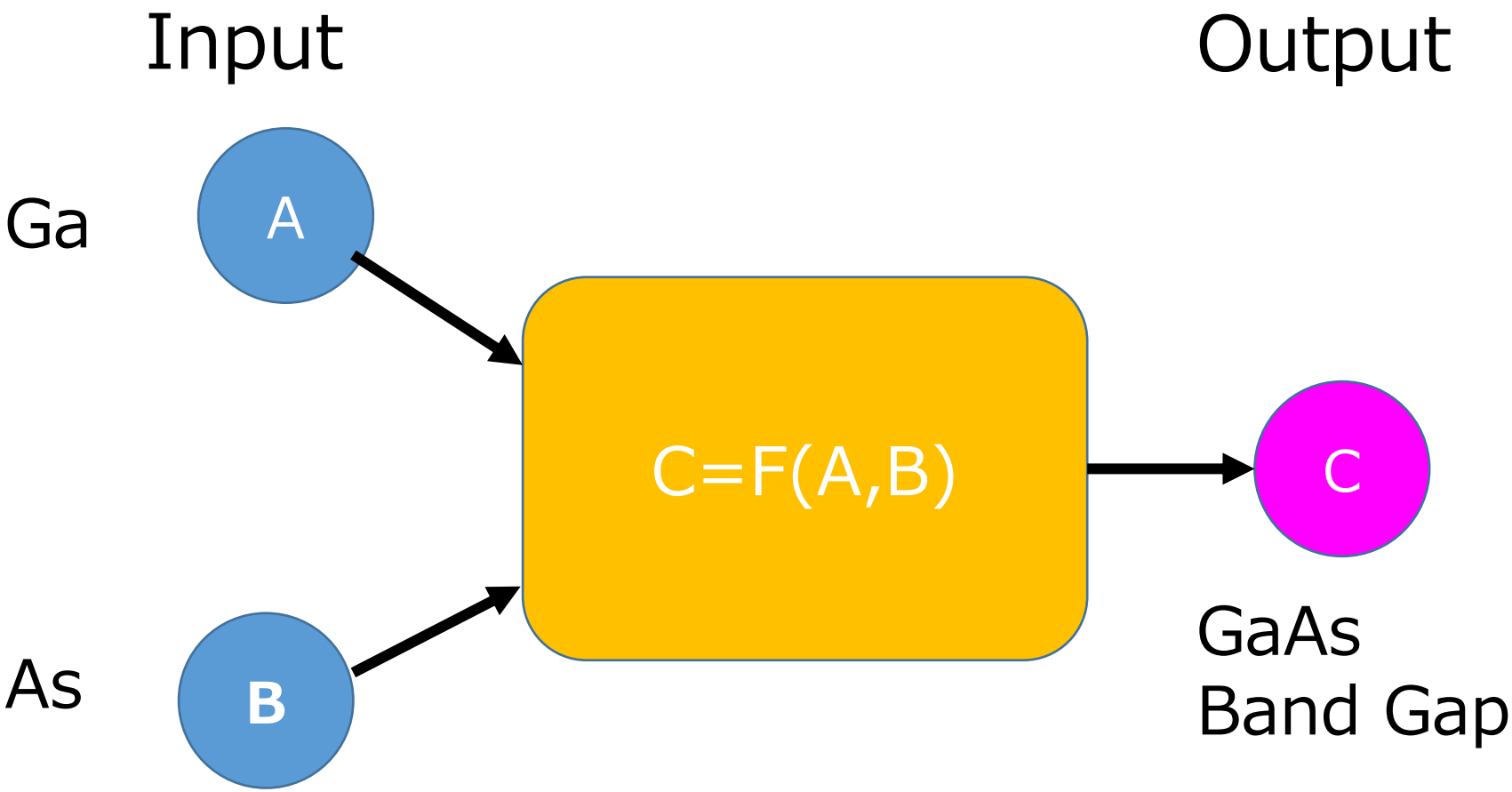
Visualization of calculated data (Magnetization and Currie Temperature)

From the data by Dr.Hiori Kino of NIMS

More than 70,000 data was calculated for quaternary metal alloys.

•Some metal alloys which contain
• Fe,Co Mn showed higher magnetic property and higher Currie temperature.

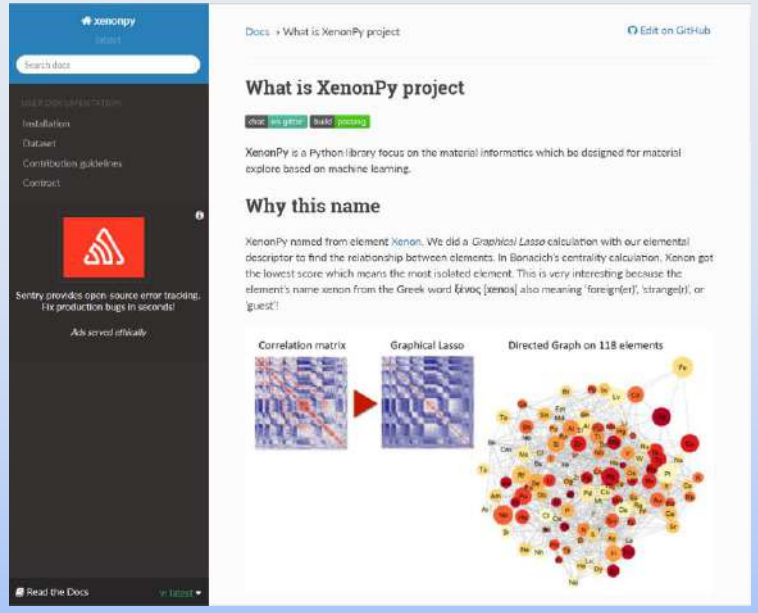
How we can use Machine Learning



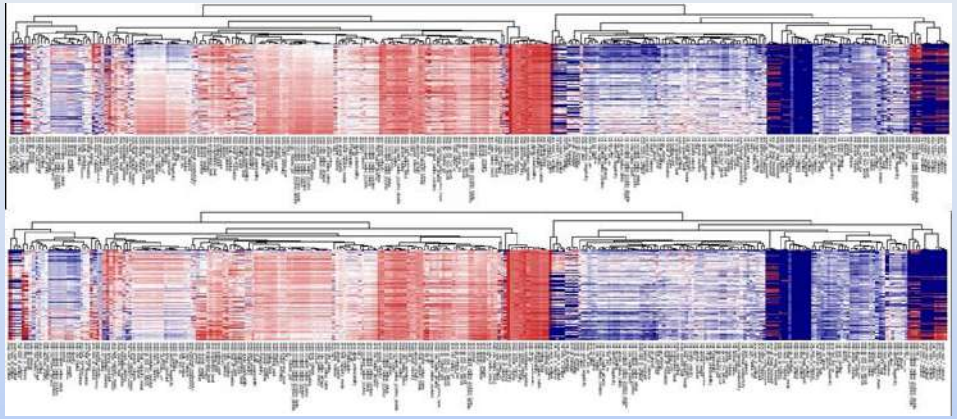
$$C = d_1A_1 + d_2B_1 + d_3A_2 + d_4B_2 + \cdots\cdots$$

$A_1\cdots$、$B_1\cdots$:Descriptors

Descriptor library for Machine learning



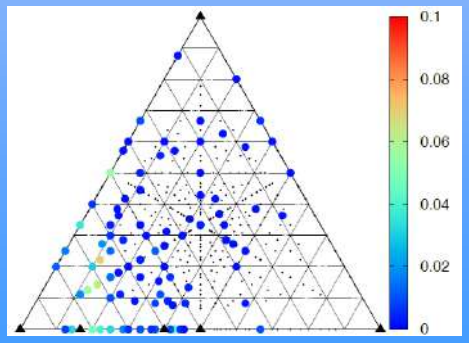
Xeon Py （Python 対応）



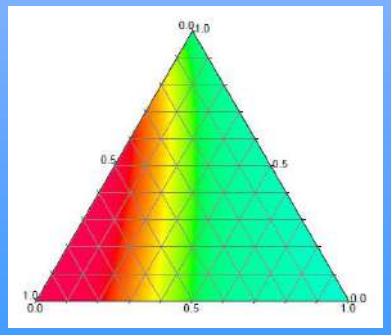
Automatic despriptor mining

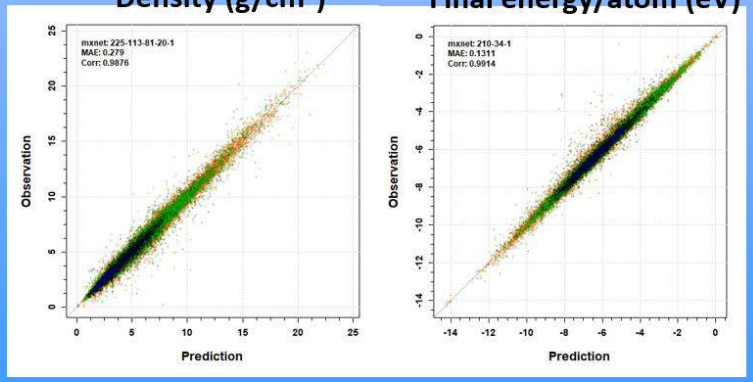
Property speculation

Structure stability



Property

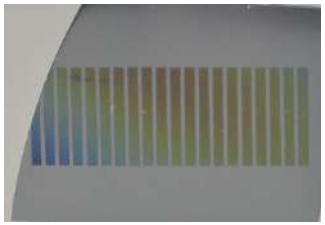


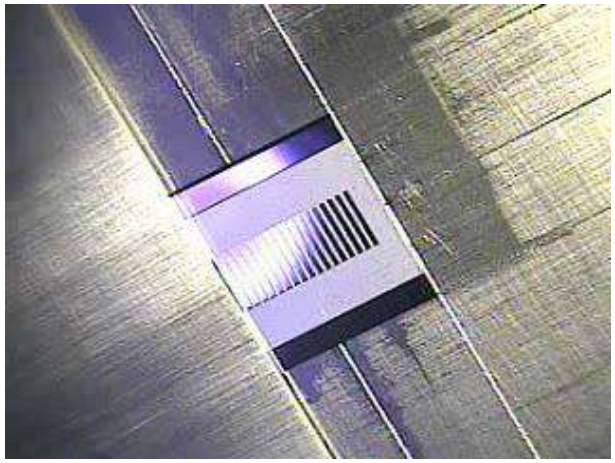


New materials discovery by ML

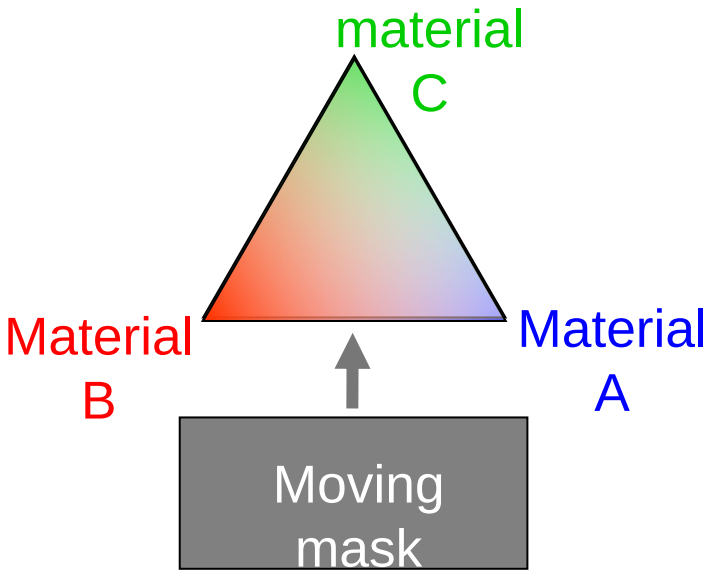
③ High Throughput Experimentation

Binary combinatorial synthesis



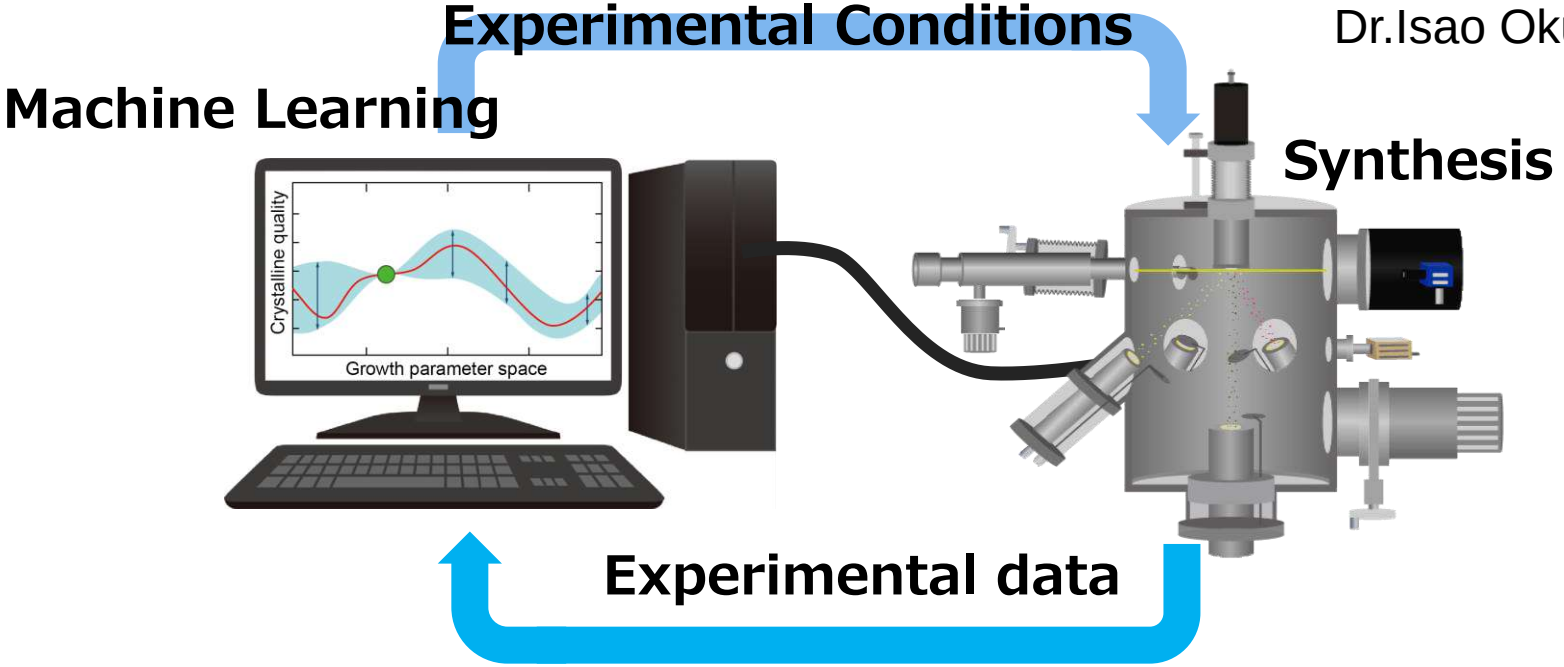


Ternary combinatorial synthesis



High throughput Synthesis supported by machine learning
-For efficient synthesis with the best condition -

Dr.Isao Okudo Data



-Automatic synthesis condition determition by Bayesian Optimization

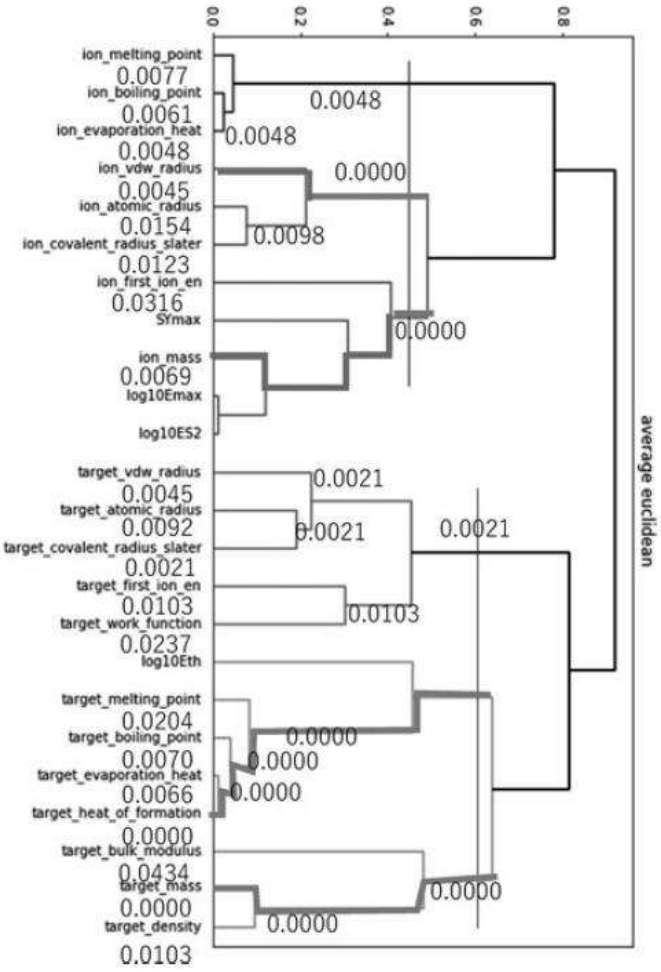
-Full closed loop system to find the condition

-One of the system which is linked to automatic characterization tools.

Process Informatics in thin film deposition

Materials Foundry

			target	ion
periodic table		atomic	Z	Z
		atomic	**mass**	**mass**
energy	thrmodynamic	crystal	melting temperature	melting temperature
		liquid	boiling temperature	boiling temperature
		gas	evaporation heat	evaporation heat
	binding energy	crystal	**heat of formation**	
real space	length	crystal	vdw radius	
		atomic	atomic radius	
			covalent radius	
	density	crystal	density	
electric energy		atomic	ionization potential	ionization potential
		crystal	work function	
incident energy				E



Theoretical parameters
(Yamamura &Tawara eq.)

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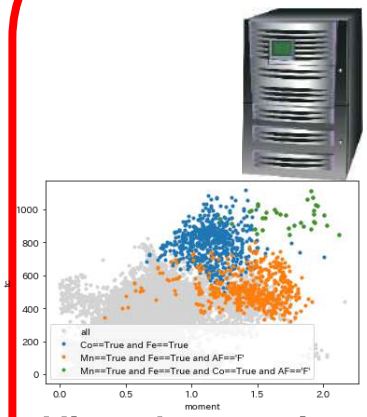
Descriptors for Machine learing

“Materials Foundry” as Smart Laboratory System

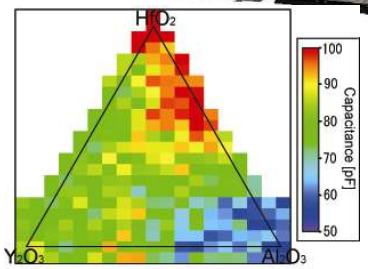
MATERIALS FOUNDRY

Smart Lab. System

Idea of Materials



Virtual screening
by Machine Learning
Deep Learning
(>10,000)



Real Screening
by automatic
high throughput
experimentaton

New Materials
Discovery

How we can handle “ Data”

NIMS Data Platform Center

M-DaC Materials Data Conversion Tools

AtomWork Adv.

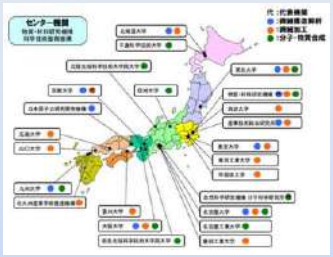
MatNavi NIMS物質・材料データベース

How the next Genereation Repository should be ?

MaDIS
NIMS MATERIALS DATA and INTEGRATED SYSTEM

Experimental data

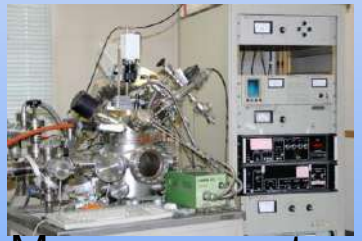
+ meta data



Experimental data from nanotech platform

Deposition (data flow)

Use (output)



Measurement data (TEM,XPS・)

+ meta data

Researchers (NIMS)

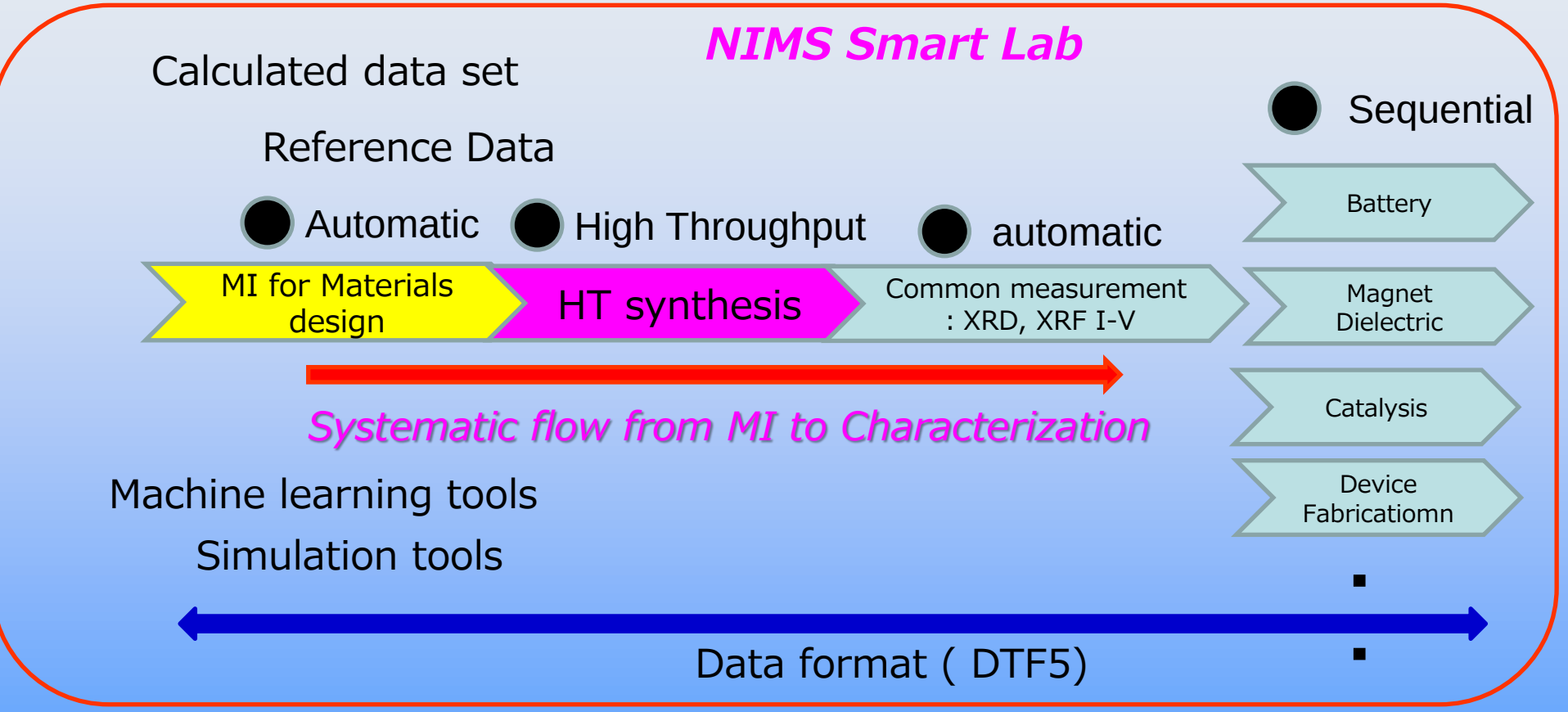
Published data (SCOPUS etc)

+ meta data

Data Plat Form Center Repository

Data Journal

“Smart Laboratory System” from MI to End: One stop Lab



Points :

- **From materials design by MI to Characterization＝＞One Stop**
- **Automation on MI, synthesis and characterization**
- **Common Data format＋data accumulation**
  ＝＞Reliable machine learning ＝＞ merit for users

Why we need “ Smart Lab. System”

Devil River

Death Valley: most Risky phase

Darwin Sea

Research phase

missing phase

Industriarizing phase

0 5-year 8-year 11-year 15-year 20-year

Stage 1 Basic R&D	Stage 2 development	Stage 3 Manufacturing technology	Stage 4 Production	Stage 5 Efficient Production

Materials Informatics → **Process Informaics** → **Smart manufacturing**

Materials Informatics
Data Driven Materials Design

Japan : NIMS Mi2i
US: MGI
China: Chinese MGI
EU: NOMAD *at al*.

Challenge: HT+AI+Procss

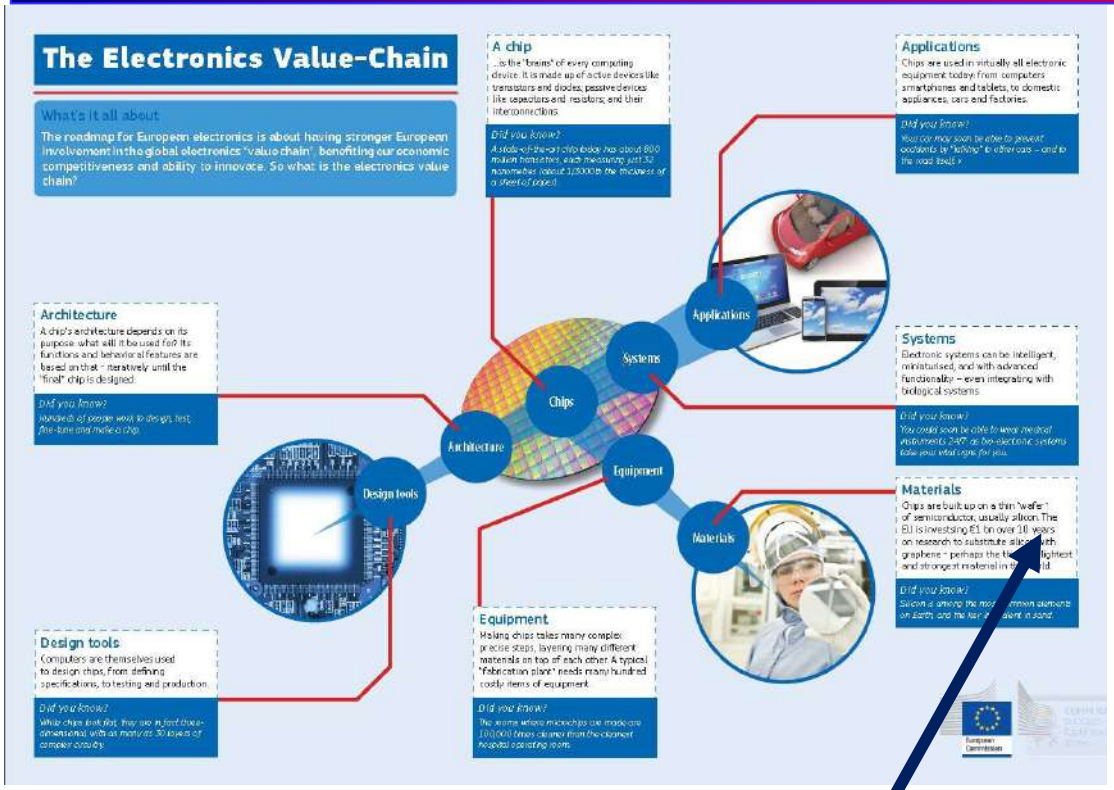
- High Throughput Experimentation
- AI supported Robotics
- AI assisted Process

Smart Lab. System

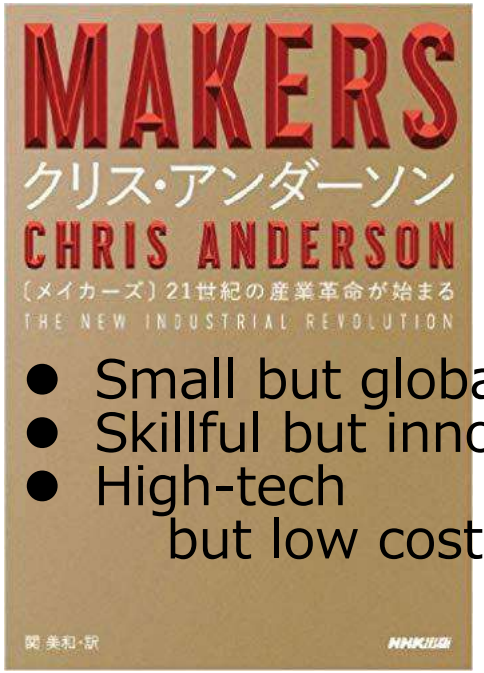
Robotics in Factory

Smart manufacturing

What comes after “ Materials Informatics”



INC11: from the Presentation of Peter Simkens

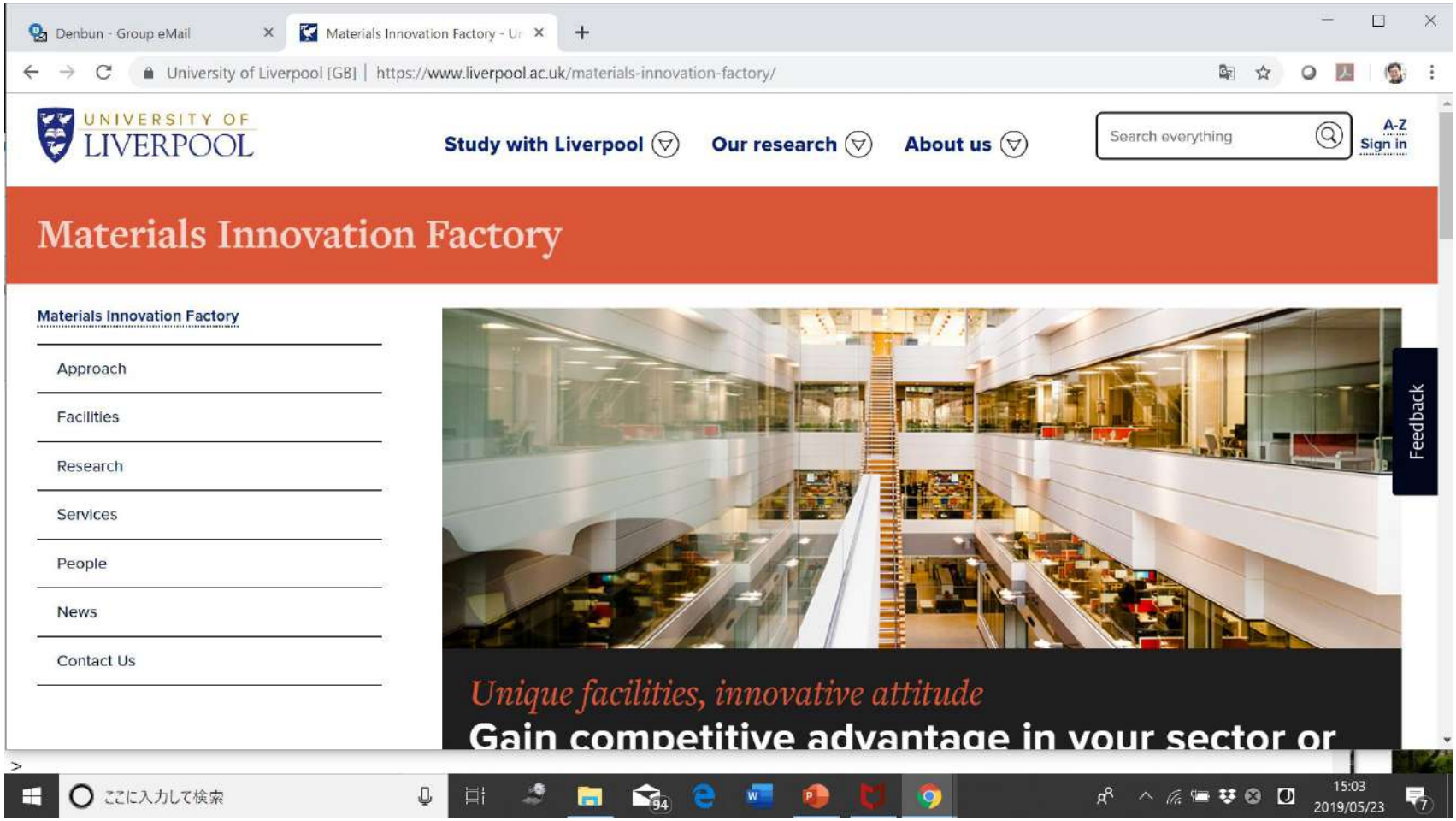


- Small but global
- Skillful but innovatie
- High-tech
  but low cost

Materials Informatics Of EU program EXCEL In HORIZON2020

- **AI**
- **Open Hardware**
- **automation**
- **cloud manufacturing**

世界の潮流１：Materials Innovation Factory at University of Liverpool



Accelerate Materials Discovery by “ Smart System”

summary

- Data driven materials science will be the major trend in materials science

- Fusion of vertical screening by MI and high throughput experimentation will accelerate new materials discovery

- Materials Informatics as a virtual screening will be developed to " Smart system" where materials design, synthesis, characterization and data storage are automatically go all out.