National Institute for Material Science

Research Trend of Data Driven Materials Research and its impact to Materials Science

Toyohiro Chikyow, Deputy Director

Center for Material Research by Information Integration (CMi2)

Materials Data Science Group
Materials Data & Integrared System (MaDIS)
National Institute for Materials Science (NIMS)

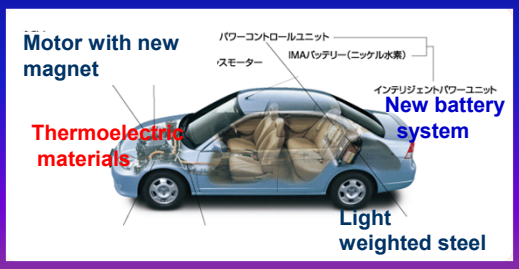
2019.9.6 CMD Workshop at Osaka Univ.

contents

- Materials Research : Past and present
- Present status of Materials Informatics
- What is " machine learning or AI" ?
- History of
  High Throughput Experimentation.
- Materials Research in future
- Conclusion

Materials innovation is the key to realize sustainable society

Super low power device and long life battery



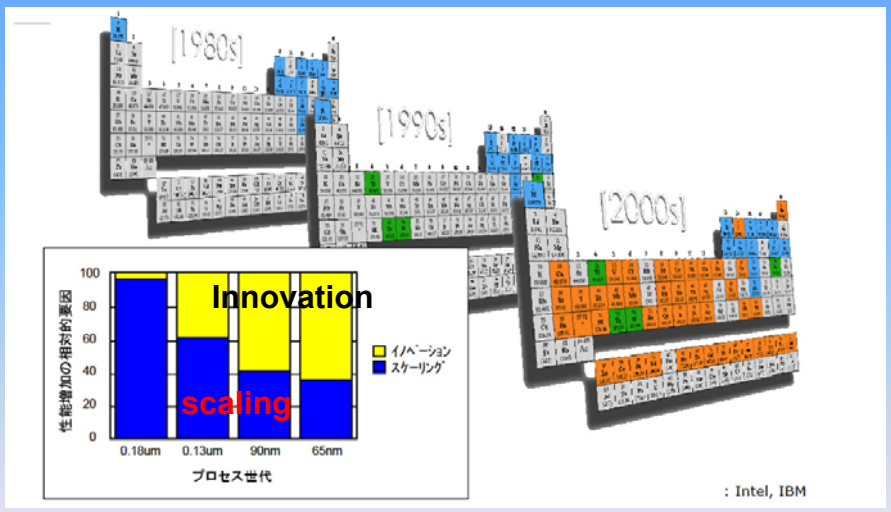
Value Chain from Materials to Products

Products

Device & system

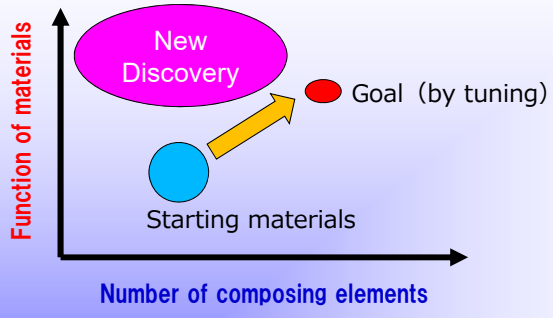
New Materials

New Materials Innovation in nano device



"Innovation" is driven by " new materials" !

Why new discovery is difficult in materials

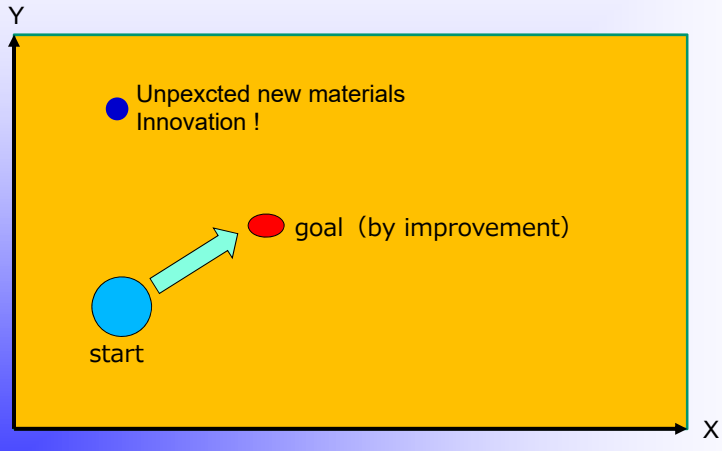


Staring Basic elements ⇒ Basic+A (A:impovement Disadvantage) ⇒ Basic+A+B (A:Improvement B:Improvement disadvantage) ⇒ Basic+A+B+C (A:Improvement B:Improvement disadvantage C:Improvement)

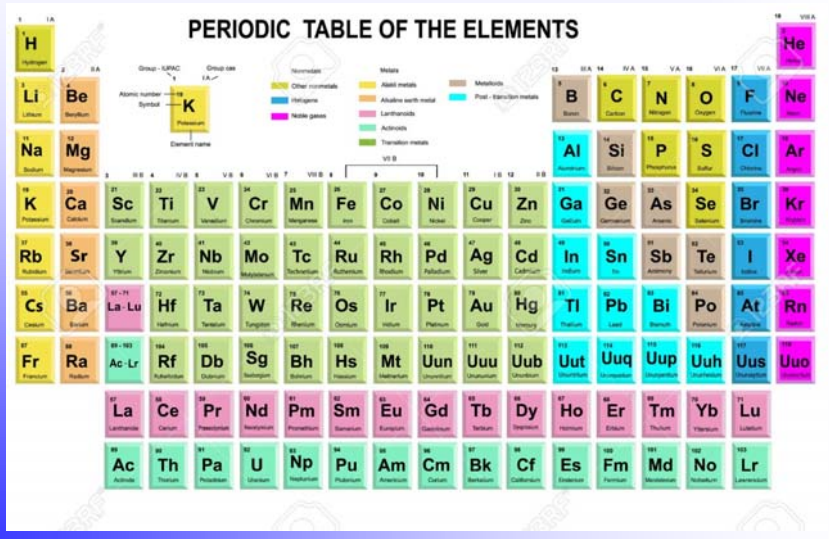
A>B>C

Extension of the Data Field& Space

National Institute for Material Science



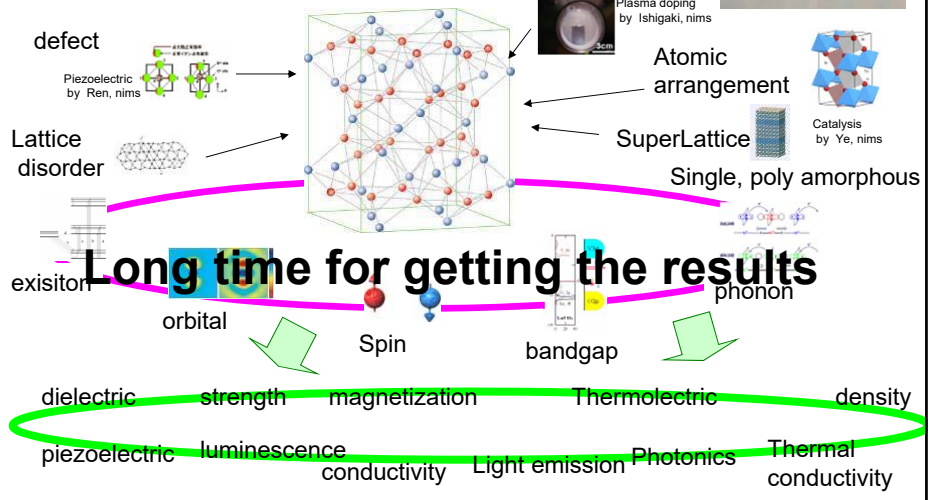
A large variety of the composition



New materials discovery by “ Computation”

Points: Materials are reviewed by “ Lattice and elements”

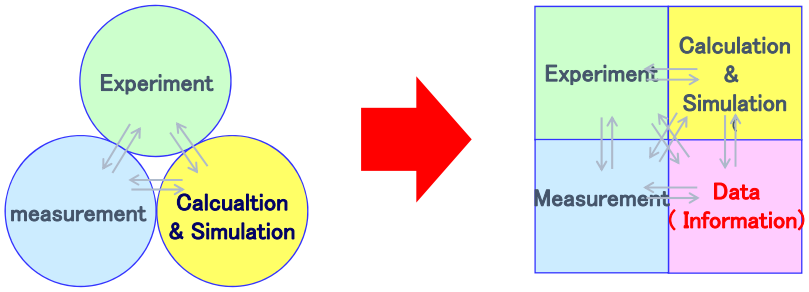
NIMS is involved in“Phase” development



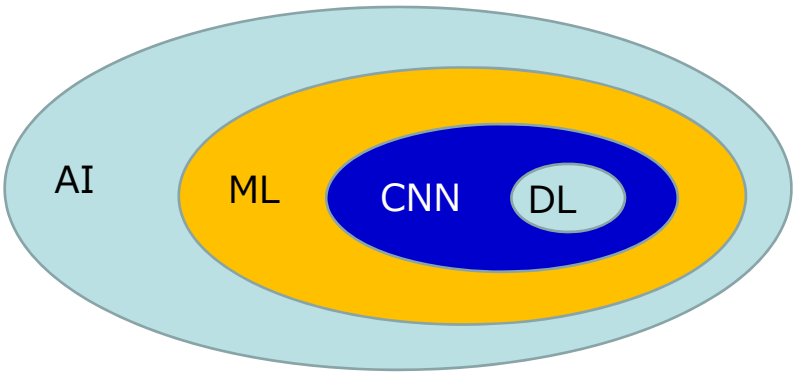
Long time for getting the results

Design new materials which does not exist before

Data Science as the 4th category

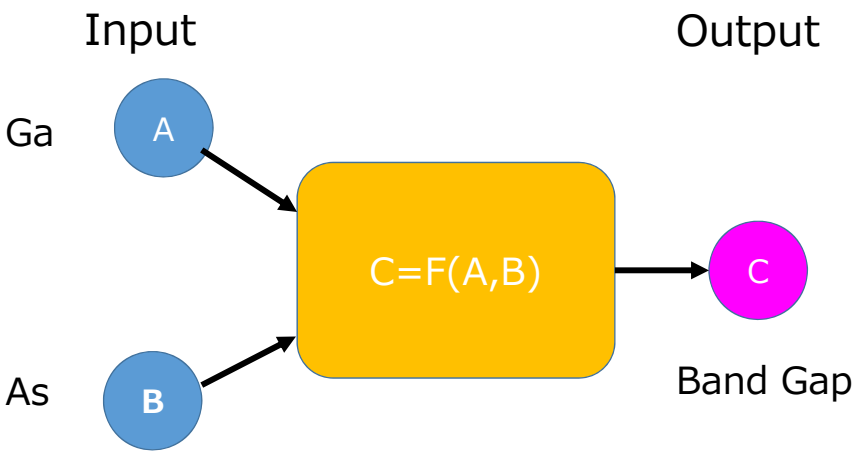


AI, ML CNN and Deep Learning



But data must be there for the AI

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

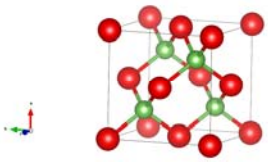
What is the descriptor ?

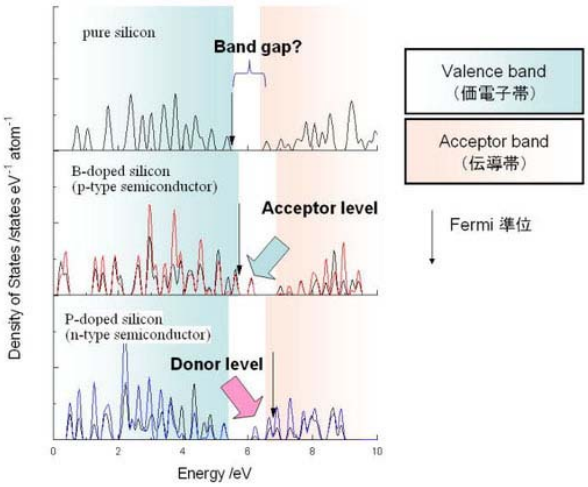
Descriptor

1) AI people:
"Just the parameter to fix the regression. No meaning"

2) Materials Informatics people:
"Those are important parameters to determine the property of the materials "

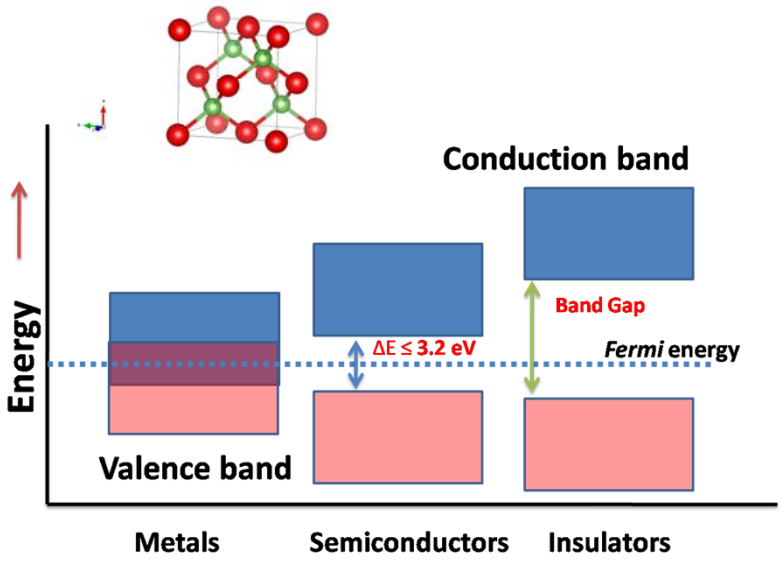
Band Gap



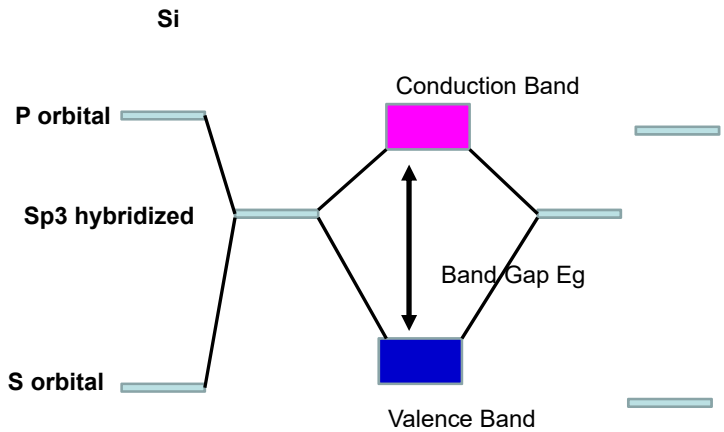


First principle calculation by Prof.Masanobu Nakayama, Nagoya Inst.of Tech

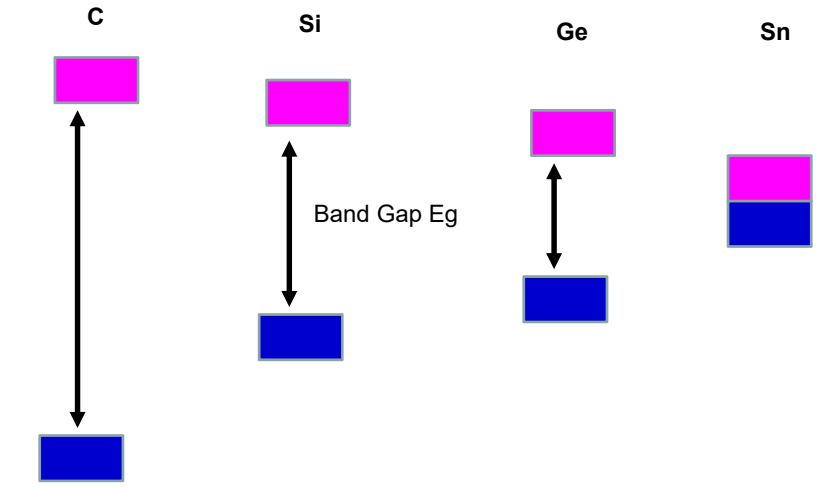
Band Gap



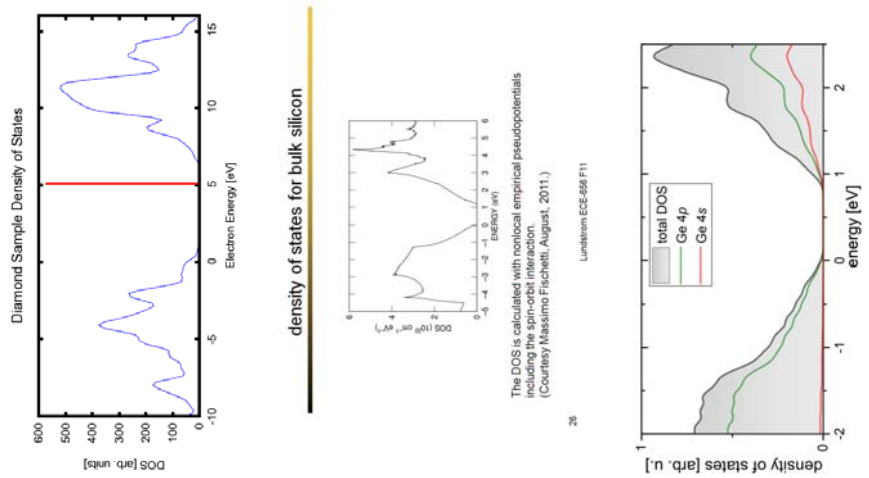
Electric Structure of Semiconductor :Si



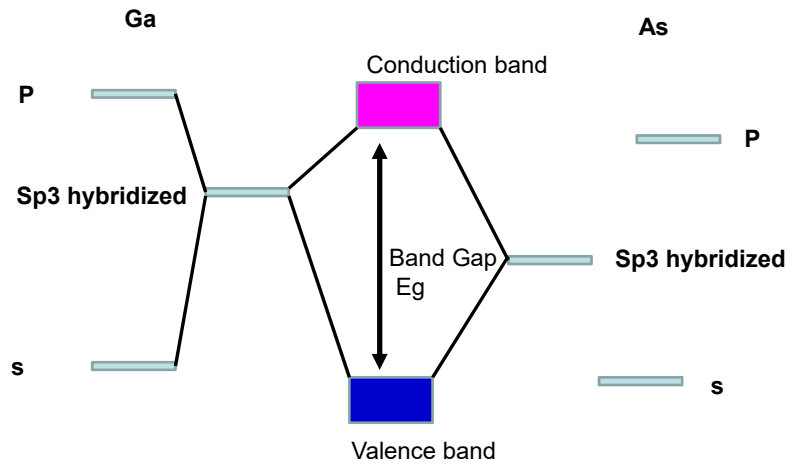
Electric Structure of Semiconductor : IV elements



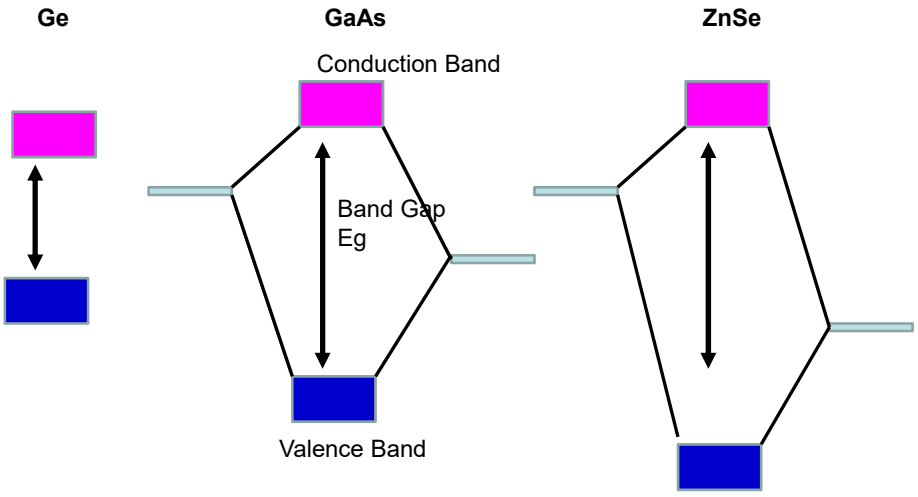
Density of States: C, Si, Ge



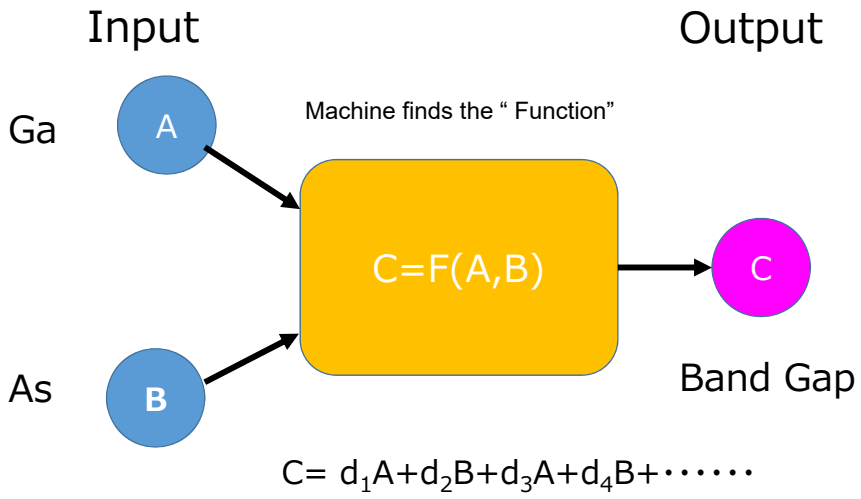
Electric Structure : GaAs



Electric Structure of Semiconductor : IV、II-V, II-VI



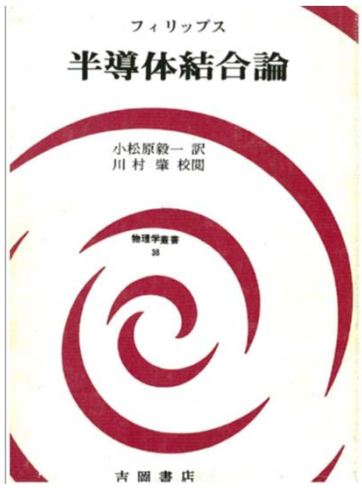
How we can know band Gap by ML



$C = d_1A + d_2B + d_3A + d_4B + \cdots\cdots$

Descriptors: atomic distance, p energy level s energy level

Schottky Barrier Height and Heat of formation



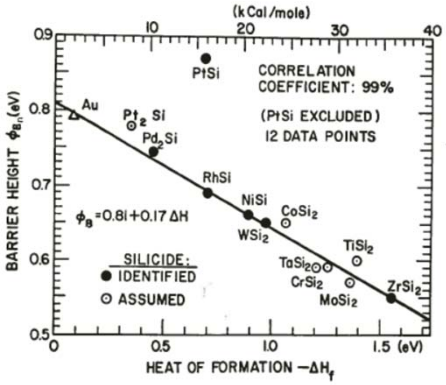


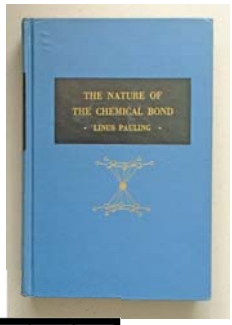
図 10.4 遷移金属珪化物－シリコン界面の障壁の高さ ϕ_{B_n} を遷移金属化合物の生成熱 ΔH_f の関数として示した.

We want to design new materials ! (Eletronegativity)

Heat of formation ΔHf ∝ X(α)－Y(β)

X(α) : Electronegativity of X :α
Y(β) :Electronegativity of Y : β

From " Nature of Chemical Bond" by Linus Poling



H 2.1																
Li 1.0	Be 1.5											B 2.0	C 2.5	N 3.0	O 3.5	F 4.0
Na 0.9	Mg 1.2											Al 1.5	Si 1.8	P 2.1	S 2.5	Cl 3.0
K 0.8	Ca 1.0	Sc 1.3	Ti 1.5	V 1.6	Cr 1.6	Mn 1.5	Fe 1.8	Co 1.8	Ni 1.8	Cu 1.9	Zn 1.6	Ga 1.6	Ge 1.8	As 2.0	Se 2.4	Br 2.8
Rb 0.8	Sr 1.0	Y 1.2	Zr 1.4	Nb 1.6	Mo 1.8	Tc 1.9	Ru 2.2	Rh 2.2	Pb 2.2	Ag 1.9	Cd 1.7	In 1.7	Sn 1.8	Sb 1.9	Te 2.1	I 2.5
Cs 0.7	Ba 0.9	La 1.2	Hf 1.3	Ta 1.5	W 1.7	Re 1.9	Os 2.2	Ir 2.2	Pt 2.2	Au 2.4	Hg 1.9	Ti 1.8	Pb 1.8	Bi 1.9	Po 2.0	At 2.2
Fr 0.7	Ra 0.9	Ac 1.1	Th 1.3	Pa 1.5	U 1.7	Np 1.3										

We want to design new materials !

Physica 100B (1980) 1–28

COHESION IN ALLOYS – FUNDAMENTALS OF A SEMI-EMPIRICAL MODEL

A. R. MIEDEMA
Philips Research Laboratories, 5600 MD Eindhoven, The Netherlands
and
P. F. de CHÂTEL and F. R. de BOER
Natuurkundig Laboratorium, University of Amsterdam, 1018 XE Amsterdam, The Netherlands

Received 7 December 1979

Table Ia

Metal	ϕ^* (V) [10, 13–15]	$n_{ws}^{1/3}$ ((d.u.)$^{-1/3}$) [10, 13–15]	$P_{m,s}^{2/3}$ (cm^2)	γ_s^0 (mJ/m^2) [6]	ΔV_m (kJ/mole) [26]
Sc	3.25	1.27	6.1	1200	6.6
Ti	3.65	1.47	4.8	2050	11
V	4.25	1.64	4.1	2600	14
Cr	4.65	1.73	3.7	2400	14
Mn	4.45	1.61	3.8	1600	4.4
Fe	4.93	1.77	3.7	2550	12
Co	5.10	1.75	3.5	2550	13
Ni	5.20	1.75	3.5	2450	12
Y	3.20	1.21	7.3	1100	7.2
Zr	3.40	1.39	5.8	1950	12
Nb	4.00	1.62	4.9	2700	18
Mo	4.65	1.77	4.4	2950	26
Tc	5.30	1.81	4.2	3050	26
Ru	5.40	1.83	4.1	3050	26
Rh	5.40	1.76	4.1	2750	23
Pd	5.45	1.67	4.3	2100	16
La	3.05	1.09	8.0	900	5.5
Hf	3.55	1.43	5.6	2200	15
Ta	4.05	1.63	4.9	3050	22
W	4.80	1.81	4.5	3300	31
Re	5.40	1.86	4.3	3650	33
Os	5.40	1.85	4.2	3500	35
Ir	5.55	1.83	4.2	3100	25
Pt	5.65	1.78	4.4	2550	18
Th	3.30	1.28	7.3[a]		
U	4.05	1.56	5.6[b]		
Pa	3.80	1.44	5.2[b]		
Cu	4.55	1.47	3.7	1850	9.3
Ag	4.45	1.39	4.7	1250	10
Au	5.15	1.57	4.7	1550	18

[a]Room temperature allotrope.

$$\Delta H = f(c)[-Pe(\Delta\phi^*)^2 + Q(\Delta n_{ws})^2]$$

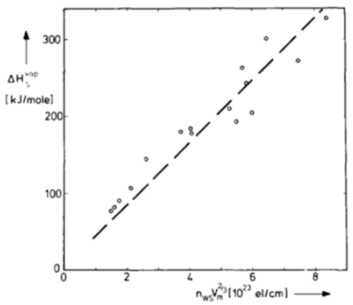
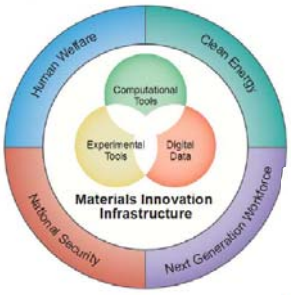


Fig. 4. The linear relation, implied by figs. 2 and 3, between the heat of vaporization per unit atomic surface, $\Delta H_s^{vap}/V_m^{2/3}$, and the electron density, n_{ws}, for non-transition metals. In this figure the divalent metals with their unusually low heat of vaporization have been omitted.

ΔHf ∝ electron density

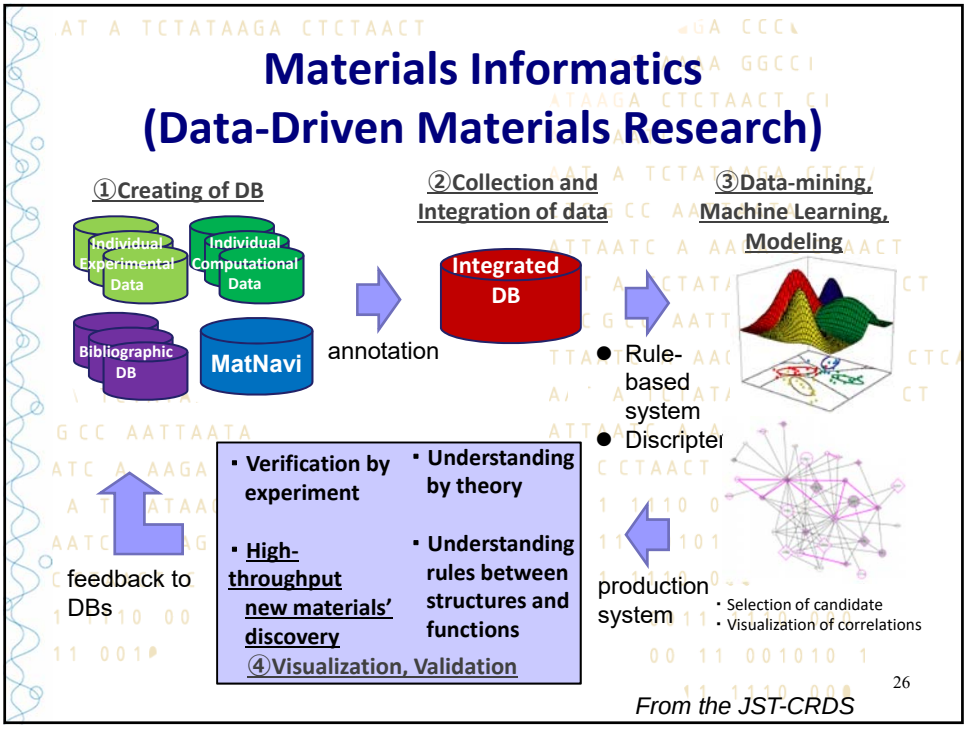
-Materials Genome Initiative-



To help businesses discover, develop, and deploy new materials twice as fast, we're launching what we call ***the Materials Genome Initiative****. The invention of silicon circuits and lithium ion batteries made computers and iPods and iPads possible, but it took years to get those technologies from the drawing board to the market place. We can do it faster.*

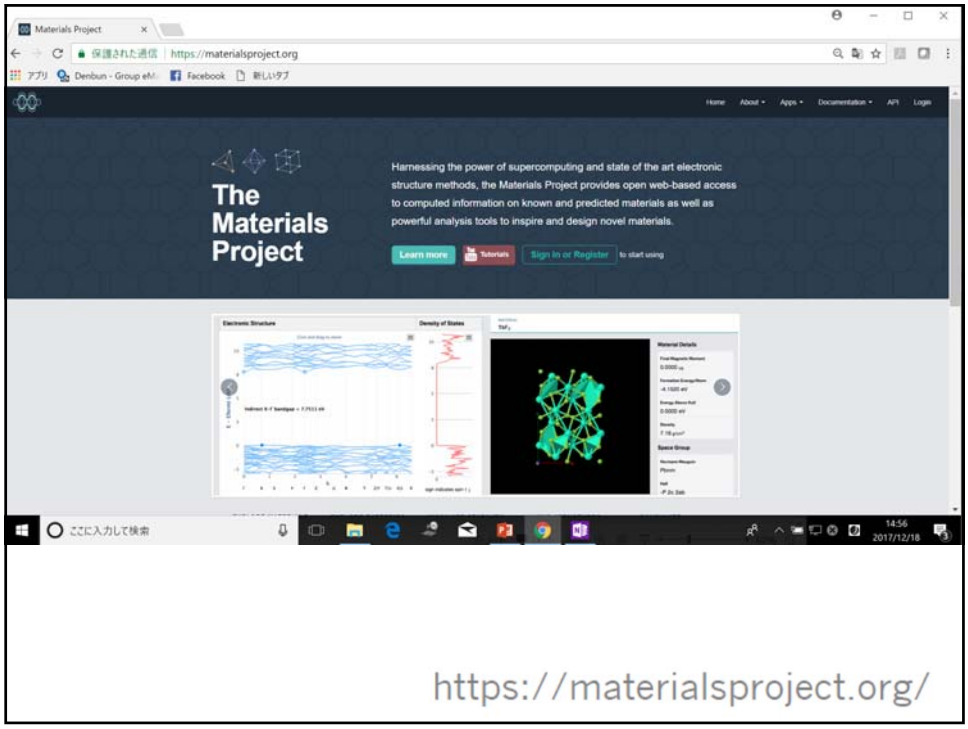
-President Obama, Carnegie Mellon University, June 2011

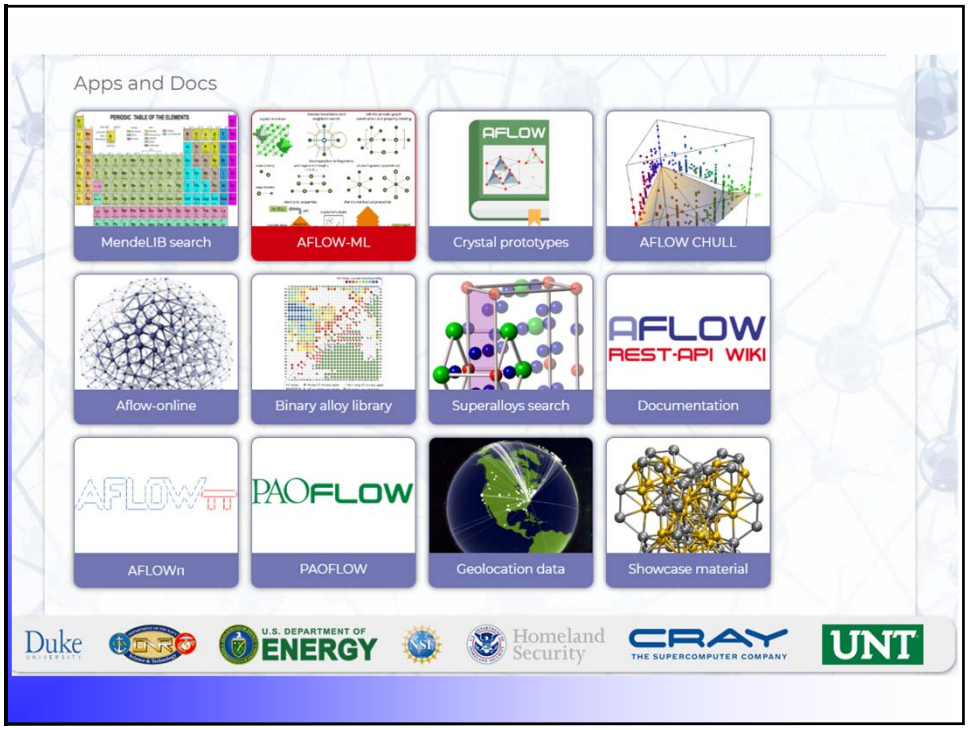
Materials Informatics (Data-Driven Materials Research)



26

From the JST-CRDS


Materials Project
https://materialsproject.org
The Materials Project
Harnessing the power of supercomputing and state of the art electronic structure methods, the Materials Project provides open web-based access to computed information on known and predicted materials as well as powerful analysis tools to inspire and design novel materials.
Learn more
Sign In or Register
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
AFLOWn
PAOFLOW
Geolocation data
Showcase material
Duke
U.S. DEPARTMENT OF ENERGY
Homeland Security
CRAY THE SUPERCOMPUTER COMPANY
UNT

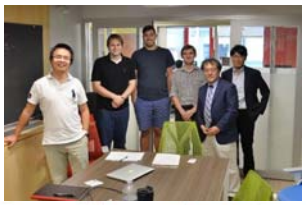
Harvard University :USA

CONFIDENTIAL

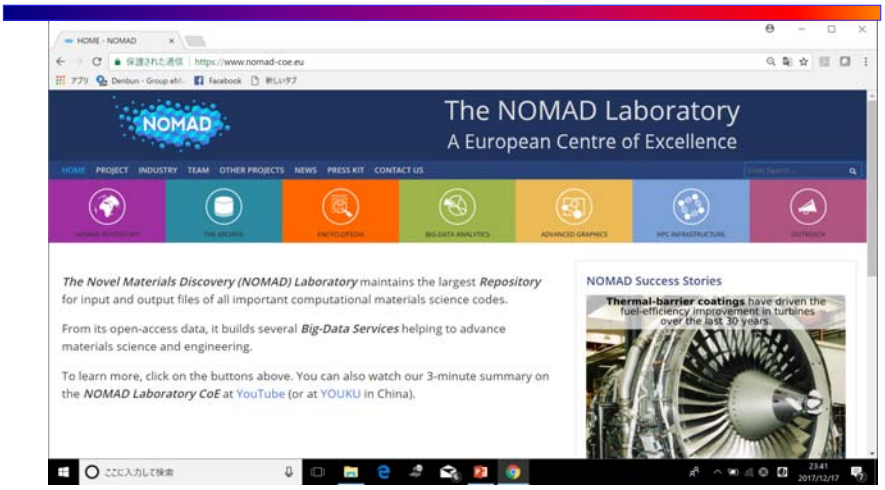
■ Clean Energy Project: Prof. Alán Aspuru-Guzik

The Clean Energy Project (CEP) is a virtual high-throughput discovery and design effort for the next generation of plastic solar cell materials.

- Organic device materials
- Calculation data



The NOMAD Laboratory
A European Centre of Excellence



CSC is part of two recently funded European Union's Horizon 2020 projects.
The NoMad (Novel Materials Discovery) project will develop "big-data analytics" for materials science. CSC's role in the project is to support the researchers in HPC code optimization and utilization of PRACE systems.

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

Two approaches to material and device development

Mi²i

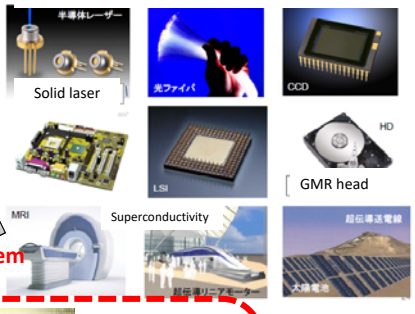
Conventional approach

Based on the fundamental physics, e.g. DFT, we investigate material properties

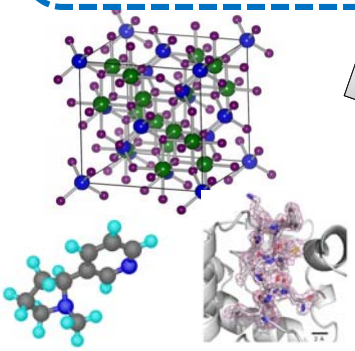
$$\left[-\frac{1}{2}\nabla^2+w(\vec{r})\right]\Phi(\vec{r})=E\Phi(\vec{r})$$

Direct problem scheme

Social and urban infrastructures are based on materials science



Inverse problem scheme



By getting help of the data science, we explore materials having a desirable properties.

Materials Informatics

National project on materials informatics
"Materials Research by Information Integration" Initiative (MI²I)

Mi²i

"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.

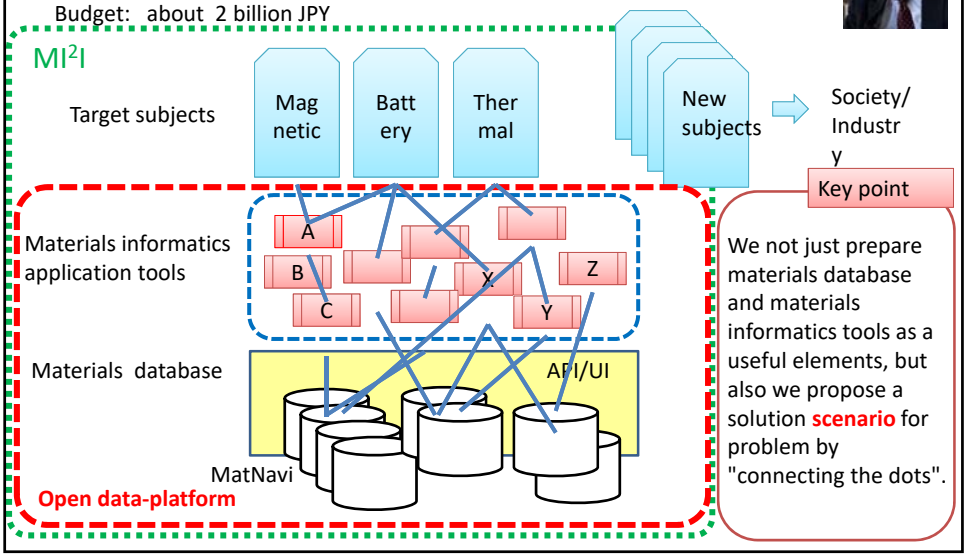
"MatNavi" provides data visualization tools and simple prediction simulator of material properties.

National project on materials informatics
"Materials Research by Information Integration" Initiative (MI²I)

Mi²i

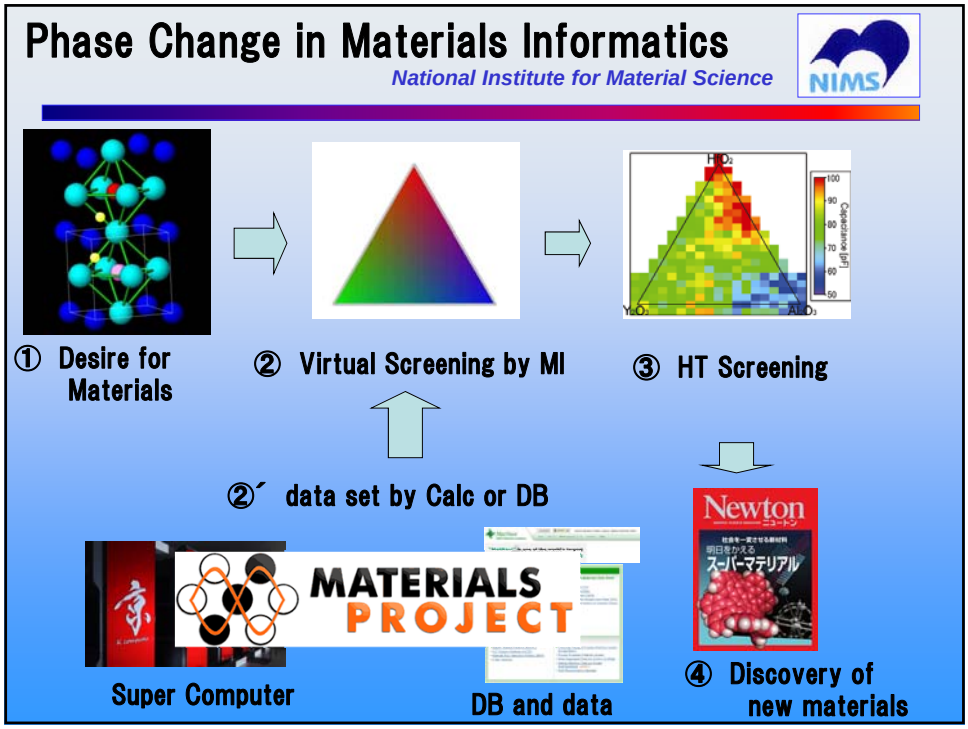
Start : July 1, 2015
Period: 5 years
Budget: about 2 billion JPY

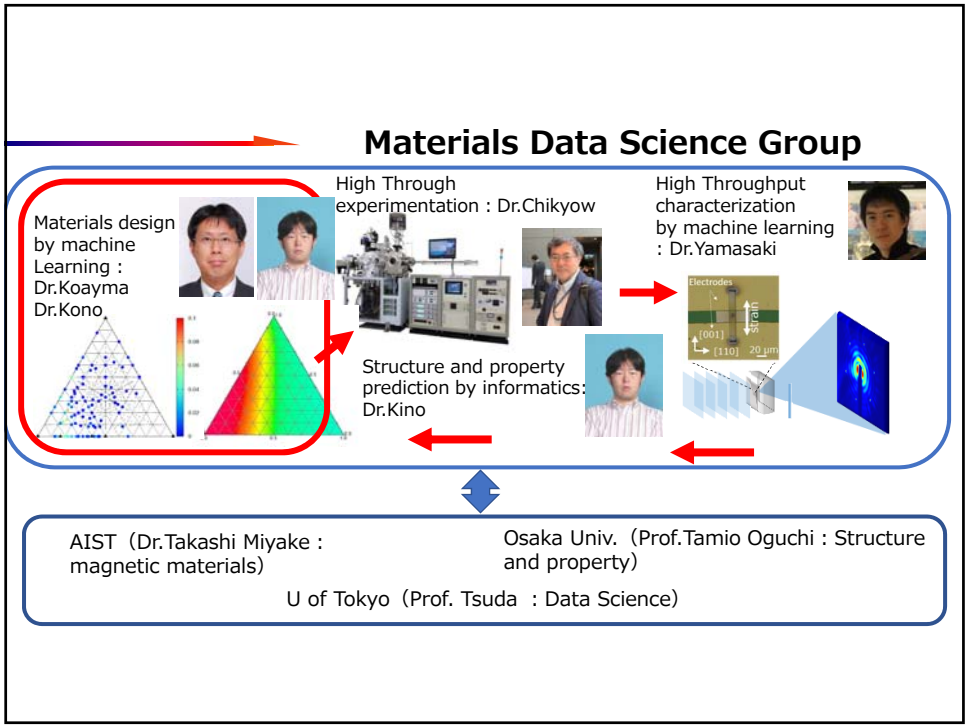
Project leader: Satoshi ITOH (NIMS)

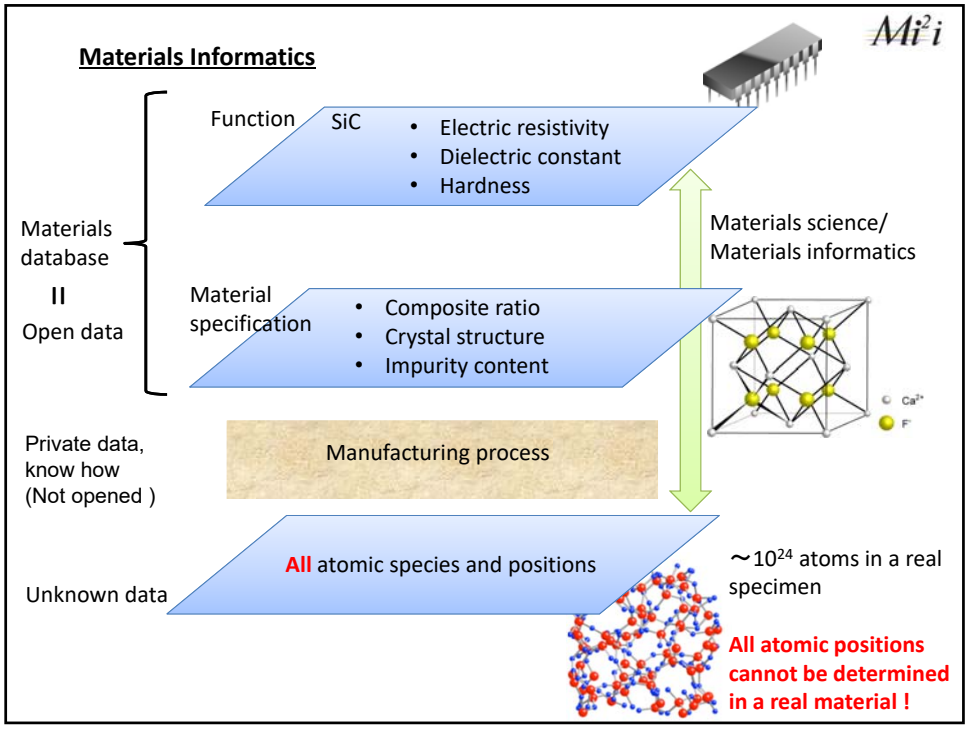


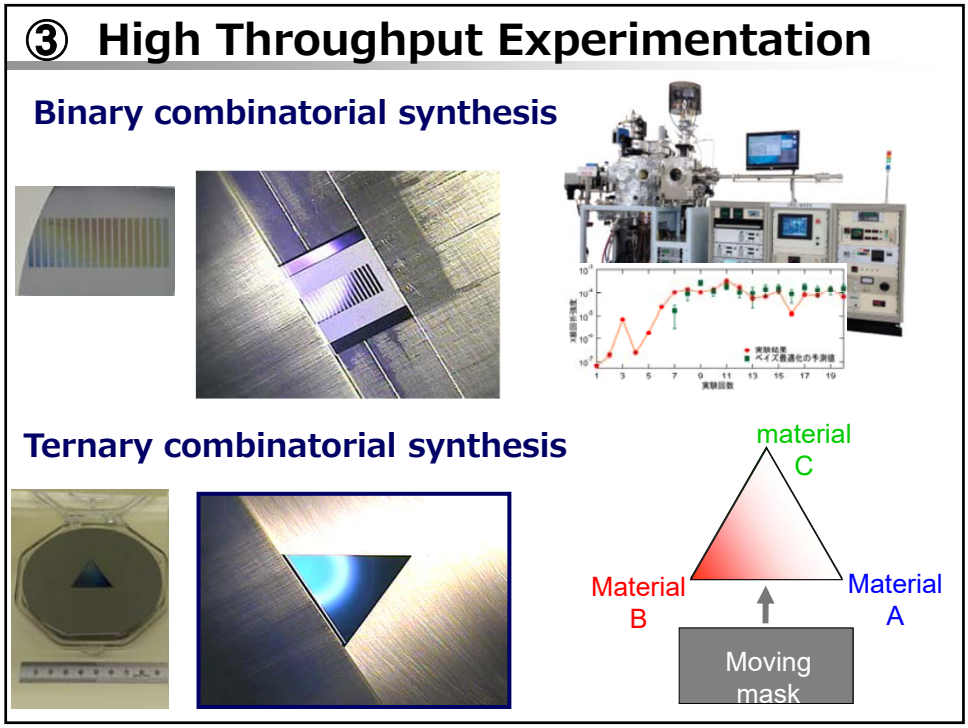
Key point

We not just prepare materials database and materials informatics tools as a useful elements, but also we propose a solution **scenario** for problem by "connecting the dots".


Phase Change in Materials Informatics
National Institute for Material Science
NIMS
① Desire for Materials
② Virtual Screening by MI
③ HT Screening
②´ data set by Calc or DB
MATERIALS PROJECT
Super Computer
DB and data
Newton
スーパーマテリアル
④ Discovery of new materials

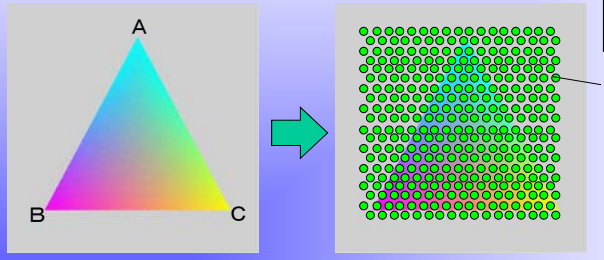

Materials Data Science Group
Materials design by machine Learning : Dr.Koayma Dr.Kono
High Through experimentation : Dr.Chikyow
High Throughput characterization by machine learning : Dr.Yamasaki
Structure and property prediction by informatics: Dr.Kino
AIST (Dr.Takashi Miyake : magnetic materials)
Osaka Univ. (Prof.Tamio Oguchi : Structure and property)
U of Tokyo (Prof. Tsuda : Data Science)


Materials Informatics
Mi²i
Function
SiC
• Electric resistivity
• Dielectric constant
• Hardness
Materials database
II
Open data
Material specification
• Composite ratio
• Crystal structure
• Impurity content
Materials science/ Materials informatics
Private data, know how (Not opened)
Manufacturing process
Unknown data
All atomic species and positions
~10²⁴ atoms in a real specimen
All atomic positions cannot be determined in a real material !


③ High Throughput Experimentation
Binary combinatorial synthesis
Ternary combinatorial synthesis
material C
Material B
Material A
Moving mask

Combinatorial I-V and C-V measurement

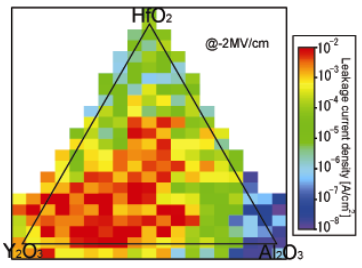
Ternary composition spread film



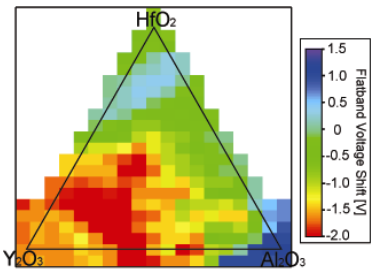
Measurement points : 500

Equipements
- Semiconductor parameter (I-V)
- LCR meter(C-V, f = 1MHz)

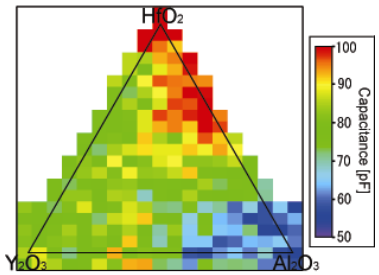
ハイスループット計測例：HfO_2-Y_2O_3-Al_2O_3 I-V, C-V測定



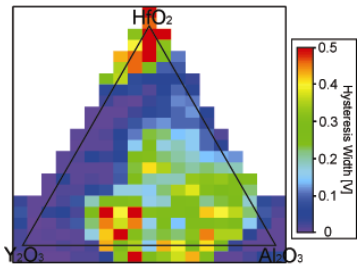
Leakage Current



Flatband Voltage Shift



Capacitance



Hysteresis Width
(film thickness:10nm)

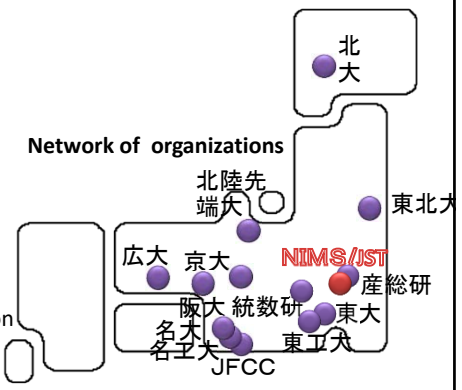
National project on materials informatics
"Materials Research by Information Integration" Initiative (MI²I)

Mi²i

Construction of "all-Japan" structure , "connecting the dots"

"all-Japan" by inter-regional cooperation
- NIMS/JST as hub organization
- Academia network・・・Hokkaido Univ., Tohoku Univ., Univ.Tokyo, TUT, JAIST, Nagoya Inst.Tech., Kyoto Univ., Osaka Univ., Hiroshima Univ., AIST, IMS, JFCC
- Translational research satellites

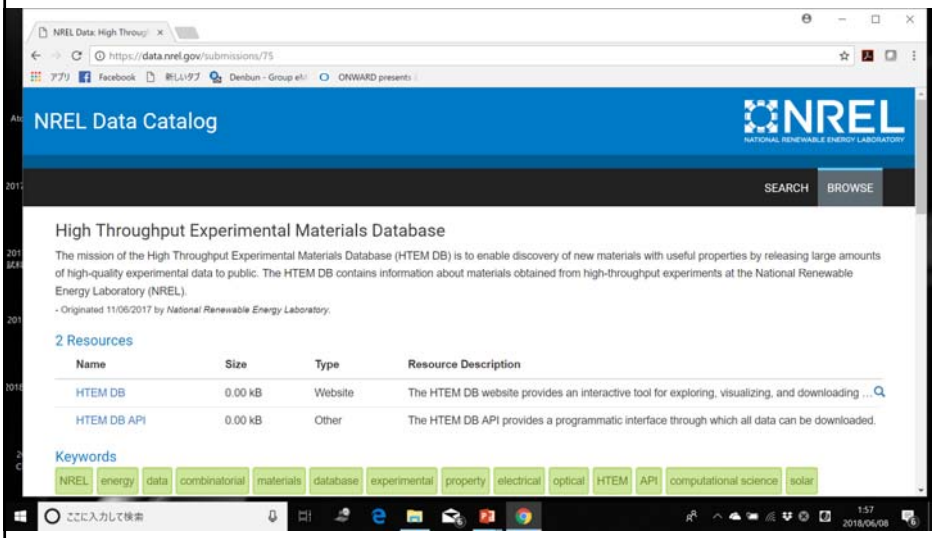
"all-Japan" by inter-sector cooperation
- Industry-government-academia cooperation
- A new scheme of multi-client collaboration



MI²I consortium (4/1/2016 ～)
- Collaboration in equal partnership of participants
- Sharing of information and achievements as possible

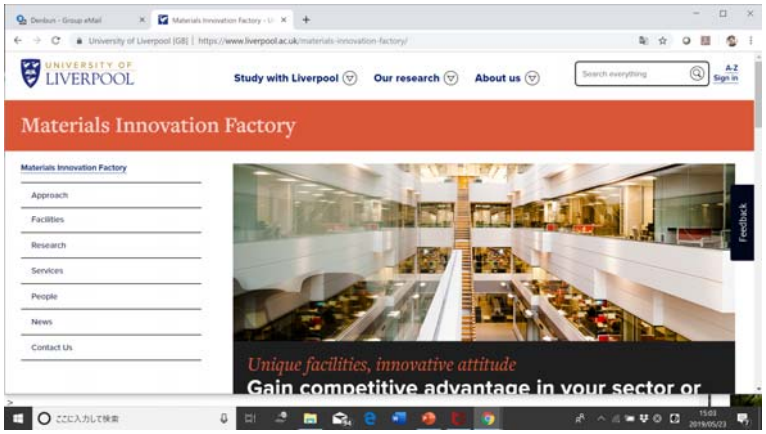
NREL : Open experimental data

秘 CONFIDENTIAL



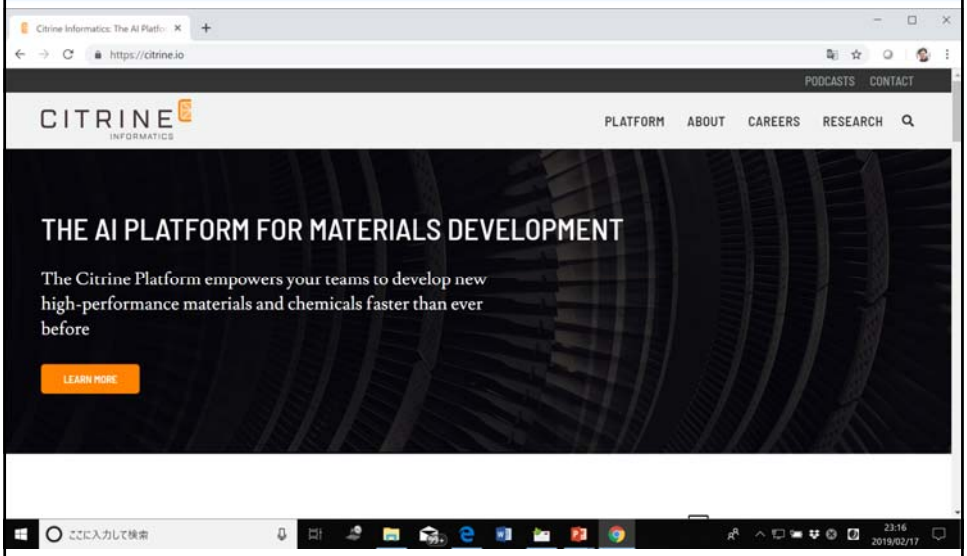
最近のトレンド：Materials Innovation Factory at University of Liverpool

秘 CONFIDENTIAL



How can collect data：Citrine

秘 CONFIDENTIAL



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
- Descriptors give us hints to think different direction
  ＝＞from “ Black box “ to “ White box”