National Institute for Material Science

# データ収集に関する研究者の取り組み、データDOIへの期待

国立研究開発法人　物質・材料研究機構
情報統合型物質・材料研究拠点
国際ナノアーキテクトニクス研究拠点（MANA）

知京豊裕

2017.3. 27　JaLC「対話・共創の場」（第3回）

# 材料開発のための２つの方法

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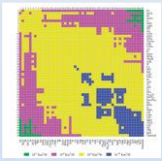
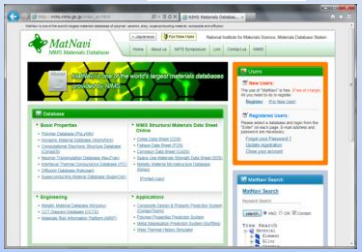
データ（選択）


帰納法



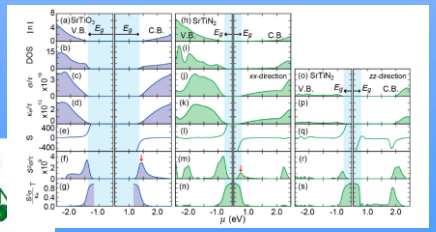



データベース

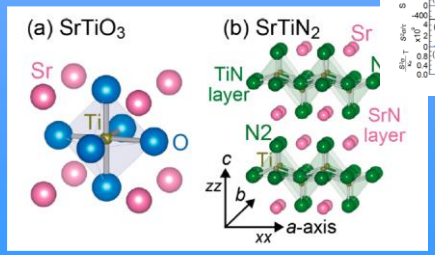
データ（蓄積）


演繹法

材料合成



材料設計





材料合成

# Materials database system : MatNavi


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

- ✓ "MatNavi" consists of about 20 database (polymer, inorganic materials, superconductivity, etc.) with high reliability.
- ✓ "MatNavi" provides data visualization tools and simple prediction simulator of material properties.

# 材料開発のため方法：自動計算

## Materials Project (MIT)

**Mission**: Accelerating materials discovery through advanced scientific computing and innovative design tools.
**Leader**(s): Prof. G. Ceder
**Budget**: -
**Collaborator**(s): LBNL, Intermolecular, Inc.

MATERIALS PROJECT

**A Materials Genome Approach**

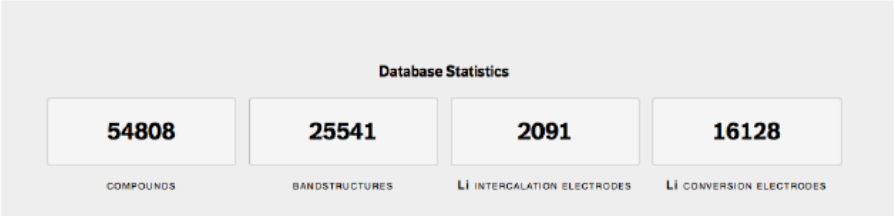
*Accelerating materials discovery through advanced scientific computing and innovative design tools.*

e.g. explore Fe2O3 or Li-Fe-O pd
Search powered by MOOGLE

**Database Statistics**

| | | | |
|---|---|---|---|
| 35840 | materials | 17219 | bandstructures |
| 497 | intercalation batteries | 16135 | conversion batteries |

（2013年12月25日クリップ）



# なぜ、実験データは少ないのか？

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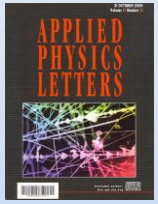
論文のデータは
データー部のみ



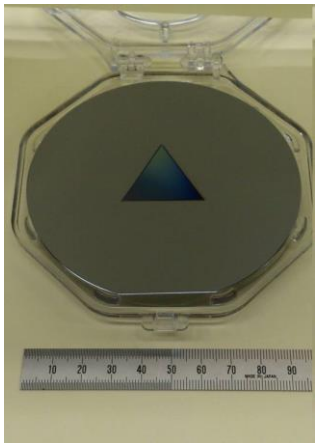

特性評価

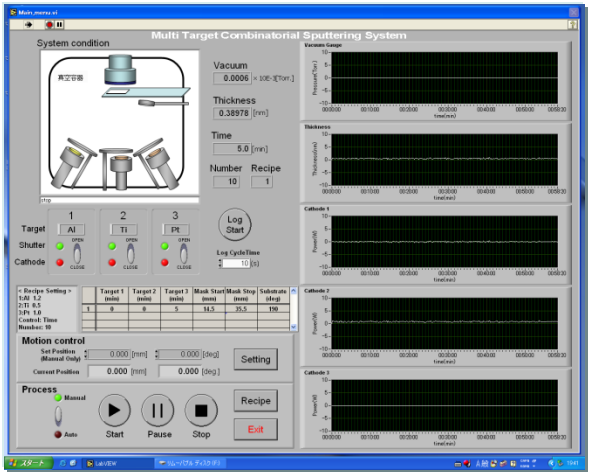
材料評価

材料合成

# High Throughput Experimentation for systematic data collection

## Multi-targets Combinatorial Sputtering system







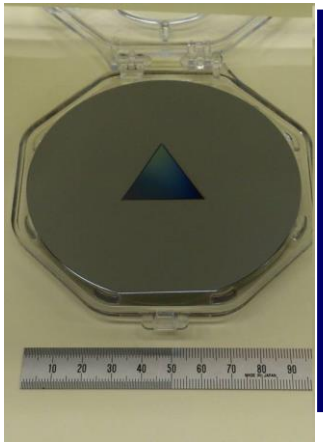
①GUI for every users

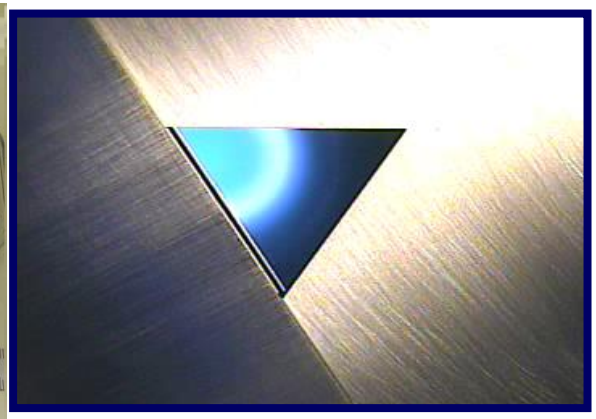
②automatic recording (date,condition, materials)

③ connection to Internet (Wireless LAN)

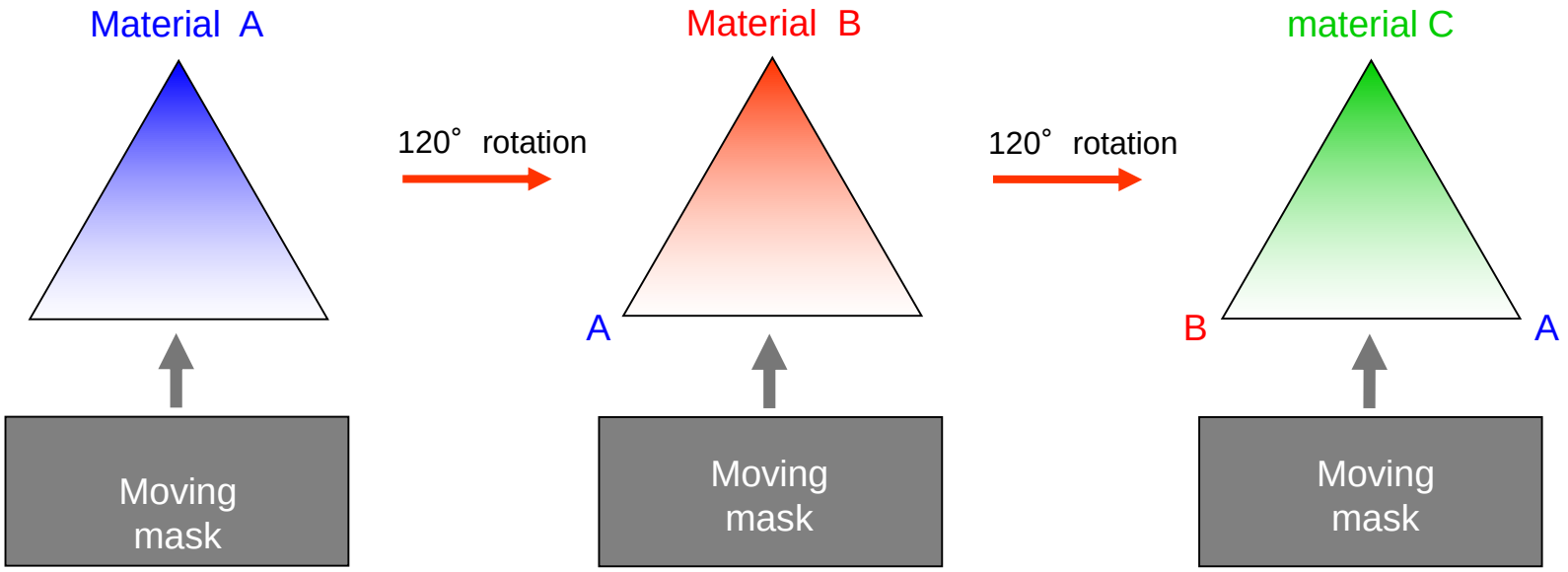
# Automatic ternary alloying by combinatorial method

## Composition spread



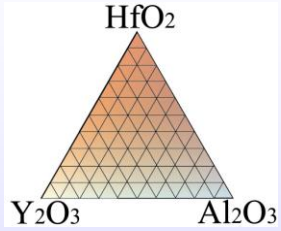


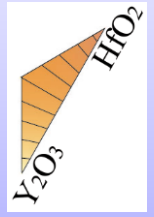
コンビスパッタ装置（コメット社製）



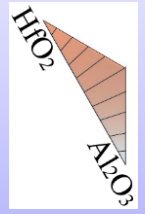

Repeat these synthesis process until getting the desired film thickness

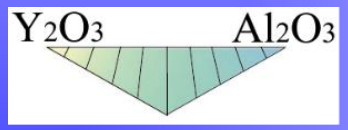
# Screening examples

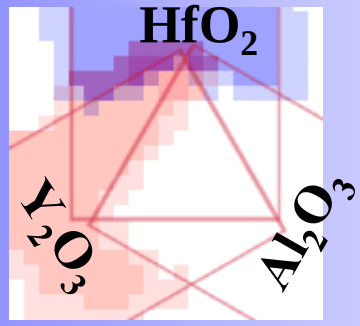




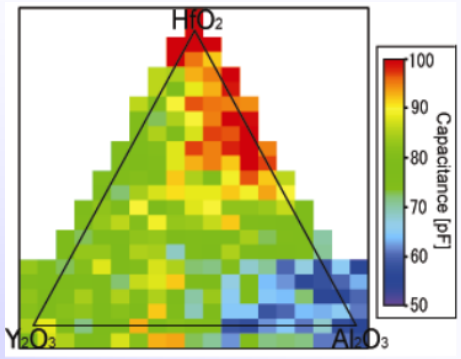


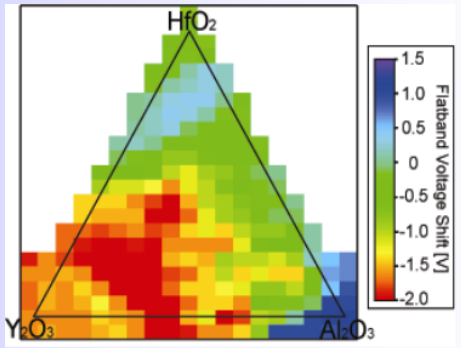




Structure mapping by XRD

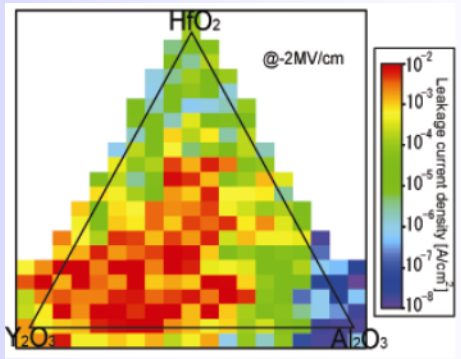
Dielectric property mapping




Flat band mapping




Leakage current mapping



# National project on materials informatics
# “Materials Research by Information Integration” Initiative (MI²I)

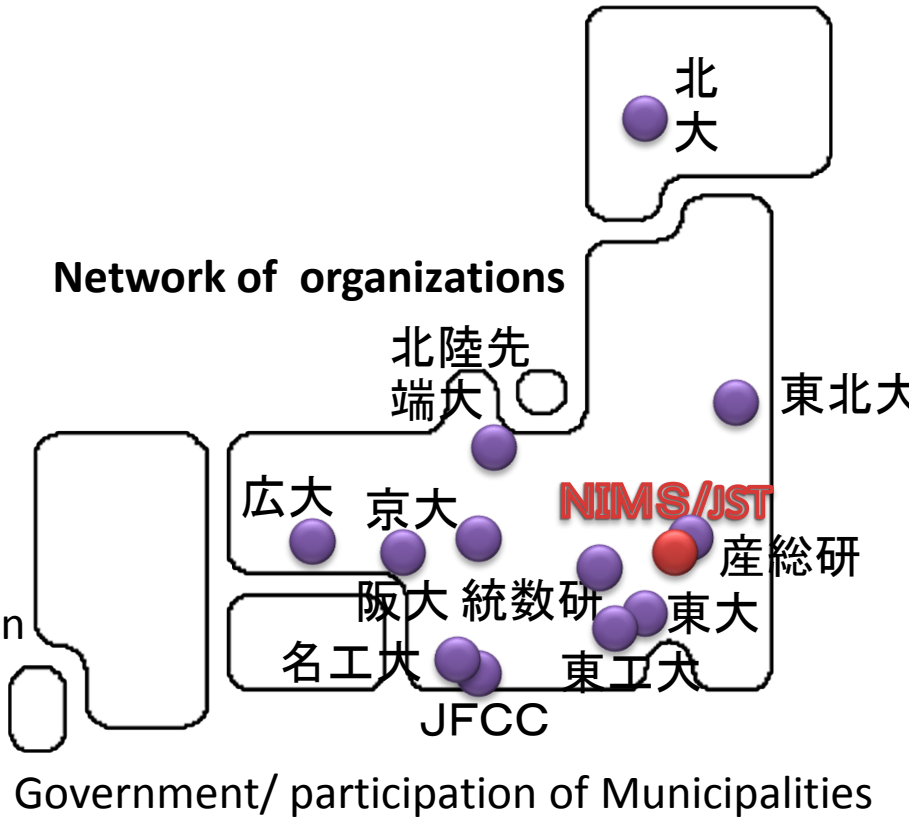
Construction of “all-Japan” structure , “connecting the dots”

“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




Government/ participation of Municipalities

MI²I consortium ( 4/1/2016 ～ )

- Collaboration in equal partnership of participants
- Sharing of information and achievements as possible

If you are interested → e-mail : mii-i@ml.nims.go.jp

**Systematic data collection !**

# なぜDOIは必要か

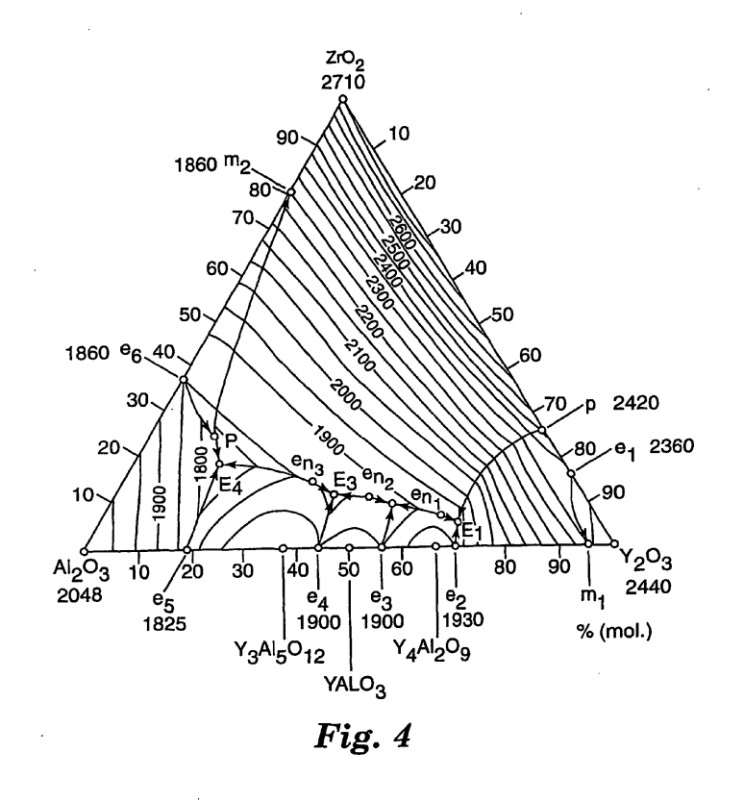
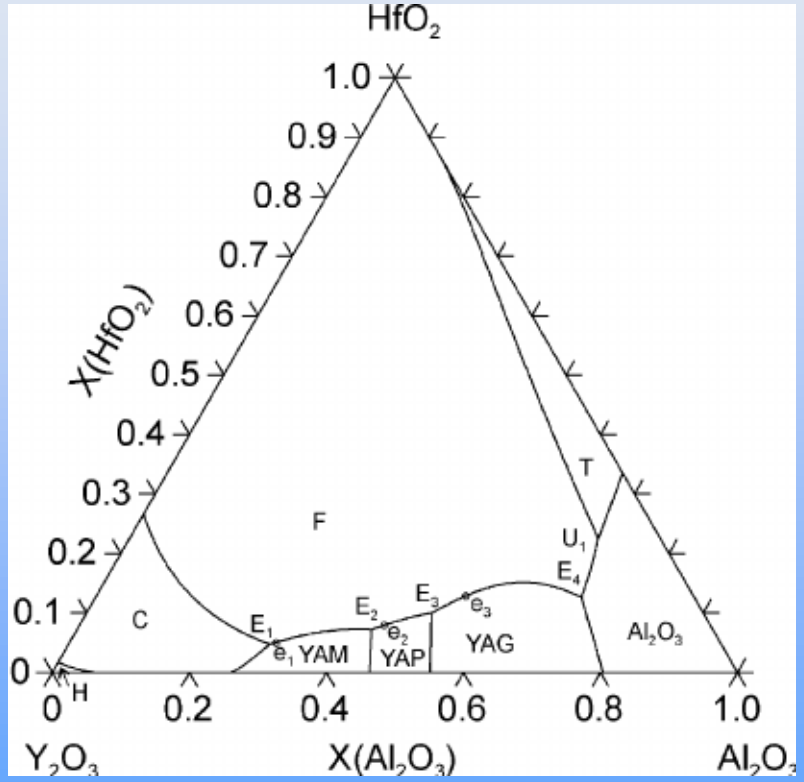



*Fig. 4*

特許から




学位論文から

**現在：データのアドレスがない。**

# データのなにが問題か？

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- 論文に載らないデータは捨てられる。
- どの装置で得たデータか不明のときがある。
- だれが作ったかも知りたい。（筆頭≠計測者）
- できれば、国際標準にしたい。

**DOIに期待。**

# Digital platform for Materials Informatics

Mi²i

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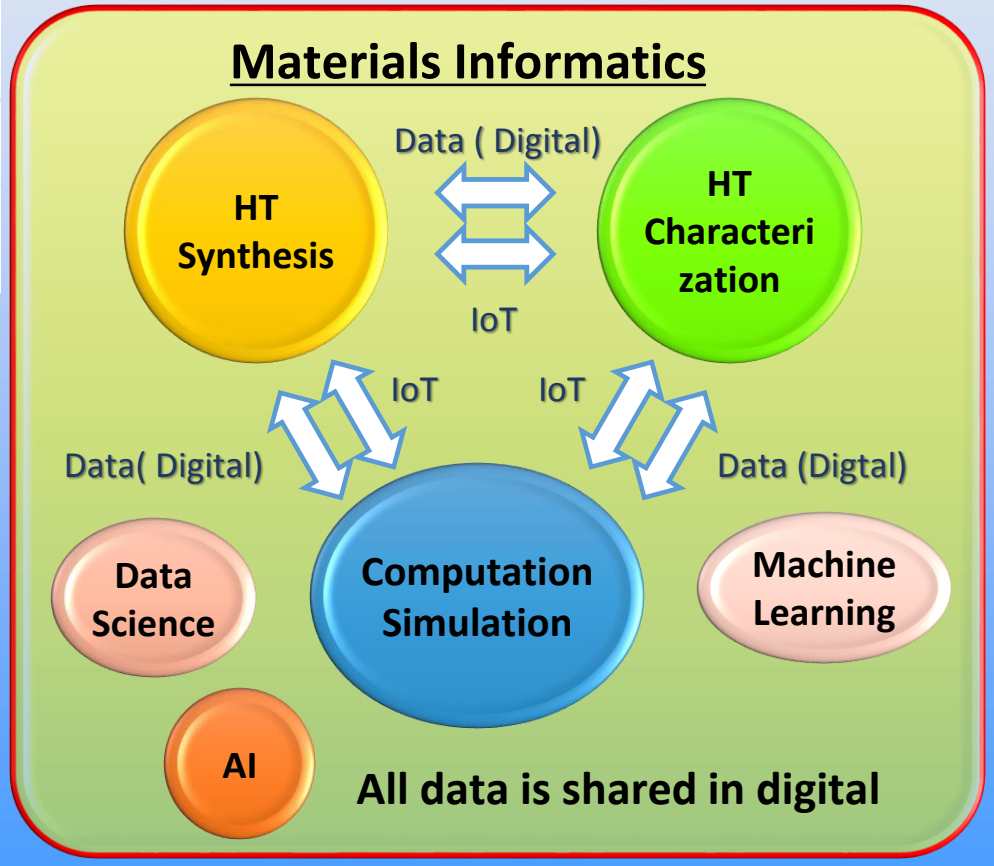
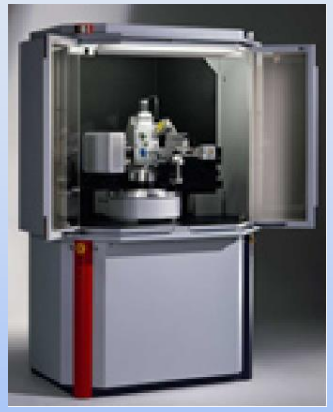
NIMS

実験装置

計算科学



評価装置
（構造）

評価装置
（特性）

# How the future materials data base is ?

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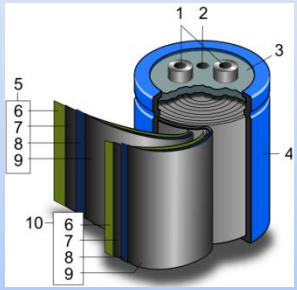
## Spicy type " visualization " in "Mat Cloud"


White paint



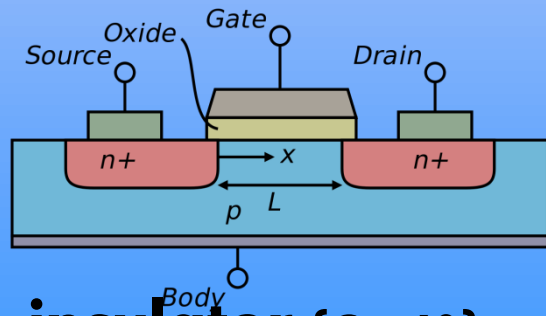

Capacitor

DSSC


UV absorption

$TiO_2$ $Al_2O_3$ $Nb_2O_5$

Transparent conductive oxide




Gate insulator (ε=60)

# データの視覚化

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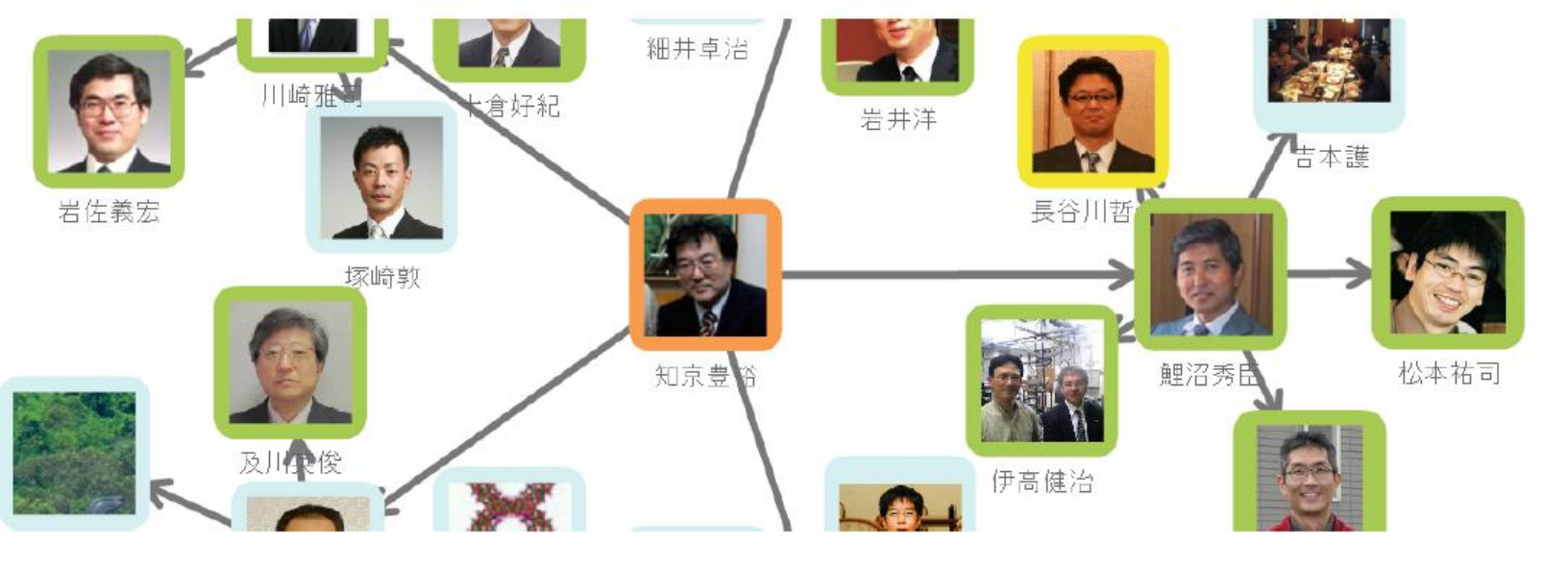
## Spicy type “ visualizing data”



# 結論

デジタル時代の材料科学のために，

- データを網羅的に集める体制
- データの関連付け
- データの視覚化

DOIはデジタル時代の材料科学に不可欠なツールとなる。