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New way to identify ceramics and glasses with tailor-made properties

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Eight Grand Challenges

Workshop on Emerging Research Areas in Ceramic Science

1. Understanding rare events in ceramic microstructures
2. Understanding the phase-like behavior of interfaces
3. Predicting and controlling heterogeneous microstructures with unprecedented functionalities
4. **Controlling the properties of oxide electronics**
5. Understanding defects in the vicinity of interfaces
6. Controlling ceramics far from equilibrium
7. **Accelerating the development of new ceramic materials**
8. Harnessing order within disorder in glasses

Challenges in Ceramic Science: A Report from the Workshop on Emerging Research Areas in Ceramic Science /
J. Am. Ceram. Soc., 95 [12] 3699-3712 (2012)

Background research

Example

Kvashnin A. et al.
New Tungsten Borides, Their Stability and Outstanding Mechanical Properties
J. Phys. Chem. Lett., **2018**, 9, 3470–3477.

Article submitted 20 April 2018

WB_5:
H_V = 45 GPa, K_{Ic} = 4 MPa·$m^{1/2}$

☹

No reference

Ma L. et al.
Preparation and sintering of ultrafine TiB_2 powders.
Ceram. Int. **2018**, *44* (4), 4491–4495.

Article available online 5 December 2017

TiB_2 + 5 wt% YAG:
H_V = 49.3 GPa, K_{Ic} = 12.68 MPa·$m^{1/2}$

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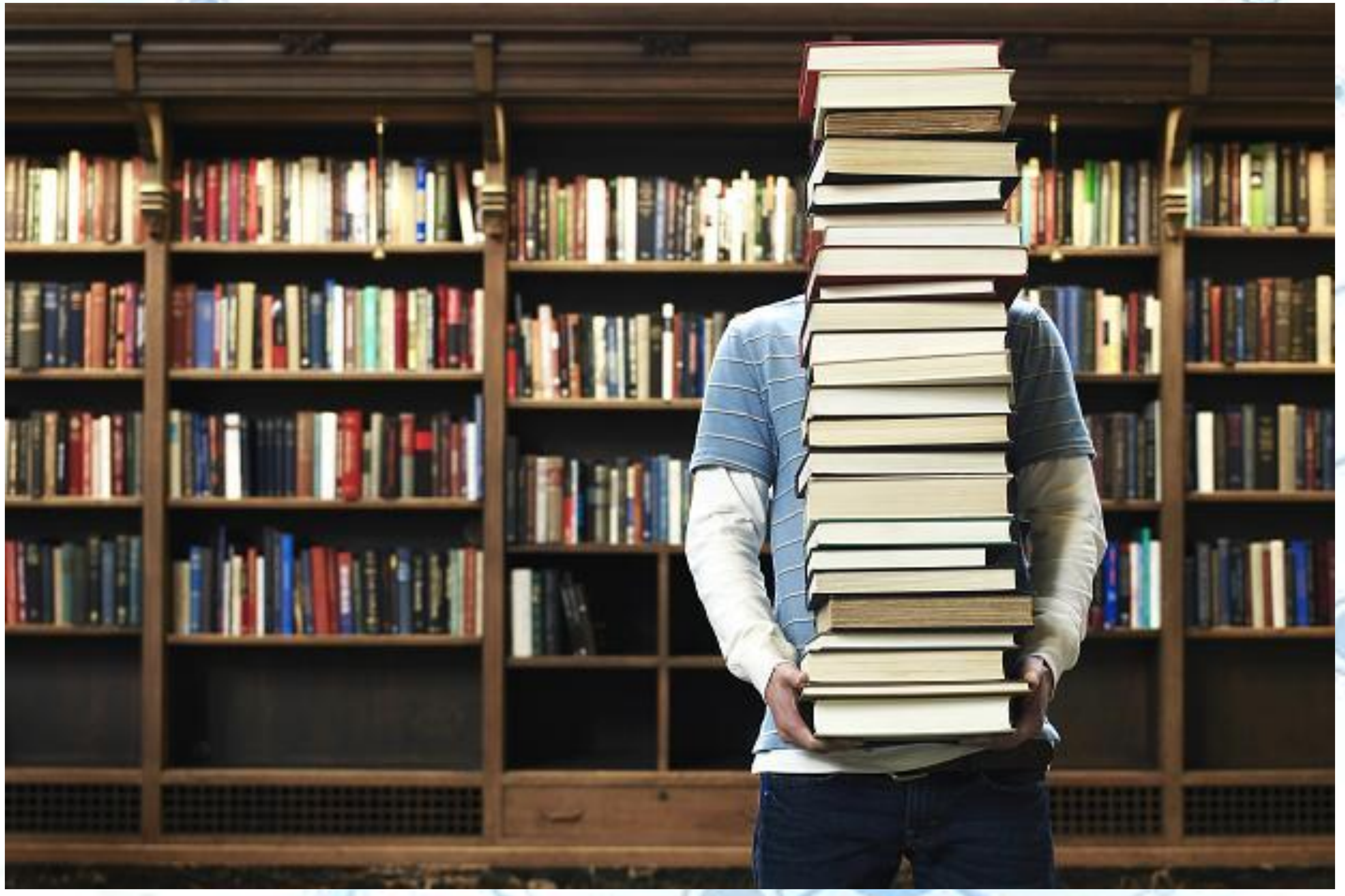
Search by material properties is very hard

A lot of handbooks should be scrutinized to find the required materials

But we will anyway miss the newly synthesized materials



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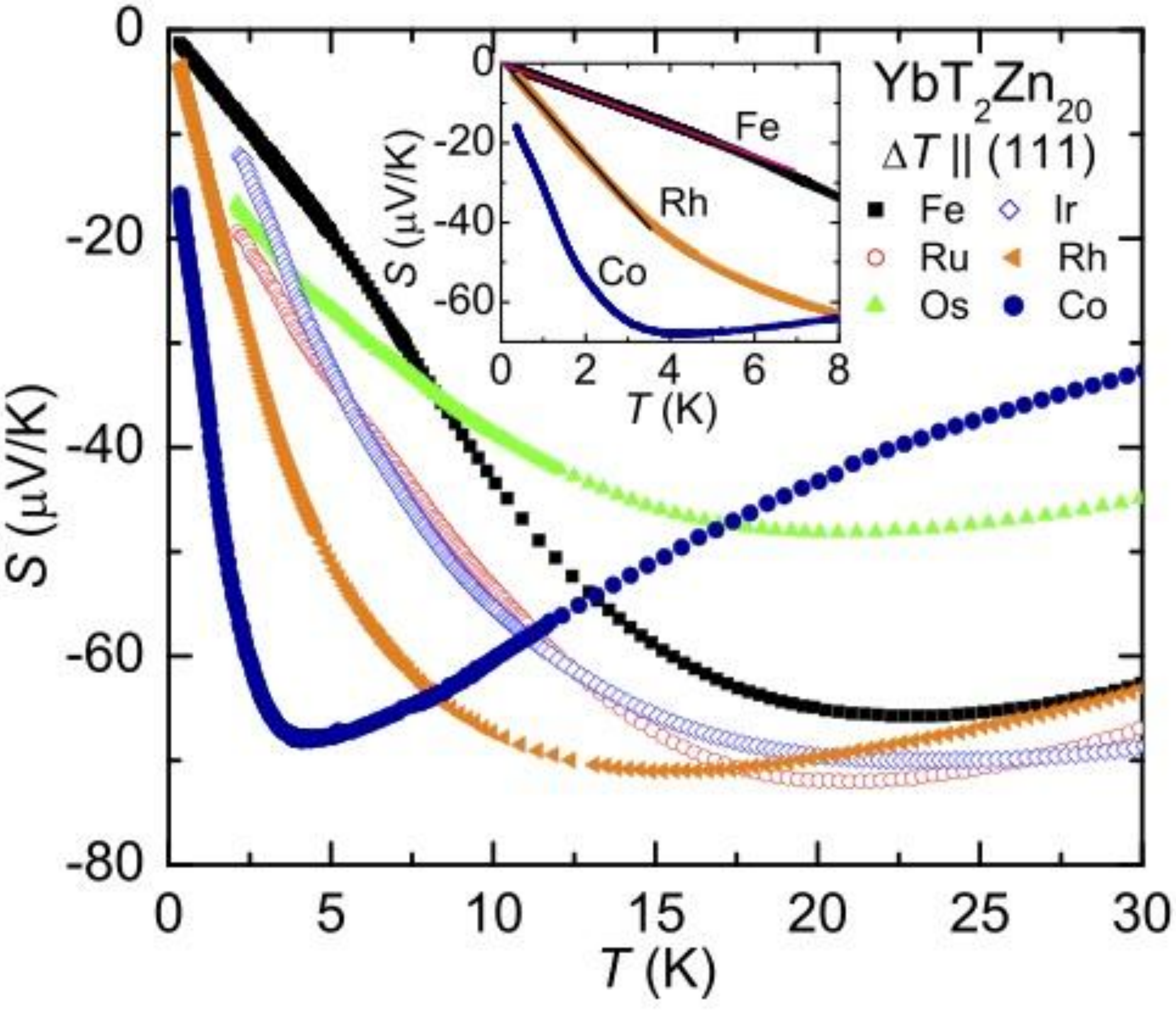
Search is even harder because of plots

Graphical information is beyond the power of search engines



New hope

Specialized databases

XIX century

Beilstein (1838-1906)
Handbook of organic compounds

Nowadays

REAXYS®

Springer Materials

SciFinder®
A CAS SOLUTION

and more ...

What is **DATA?**

Data is a set of values of qualitative or quantitative variables.

Data is measured, collected and reported, and analyzed, whereupon it can be visualized. Experimental data is data that is generated within the context of a scientific investigation by observation and recording.

Why do we need **THE DATA?**

THEY ARE USED BOTH IN SCIENTIFIC RESEARCH AND BUSINESS.

- to make decisions
- create something new
- re-develop existing products
- understand the current state of the art
- offer enterprise-wide insights
- perform risk analysis

BIG DATA
What is it?

Big data is data sets that are so voluminous and complex that traditional approaches are inadequate to deal with them.

Big data challenges include data mining, data storage, data analysis, search, sharing, transfer, visualization, querying, and updating. There are three dimensions to big data (three “V”) known as Volume, Variety and Velocity.

RAW DATA

Raw data are the source for data mining.

Data mining is a process of cleaning and capturing the data. Problems of raw data: they are unstructured, disordered and complicated. They have a lot of noise (useless data). The bigger the volume of raw data, the harder they are cleaned and mined.

Imagine a really huge supermarket

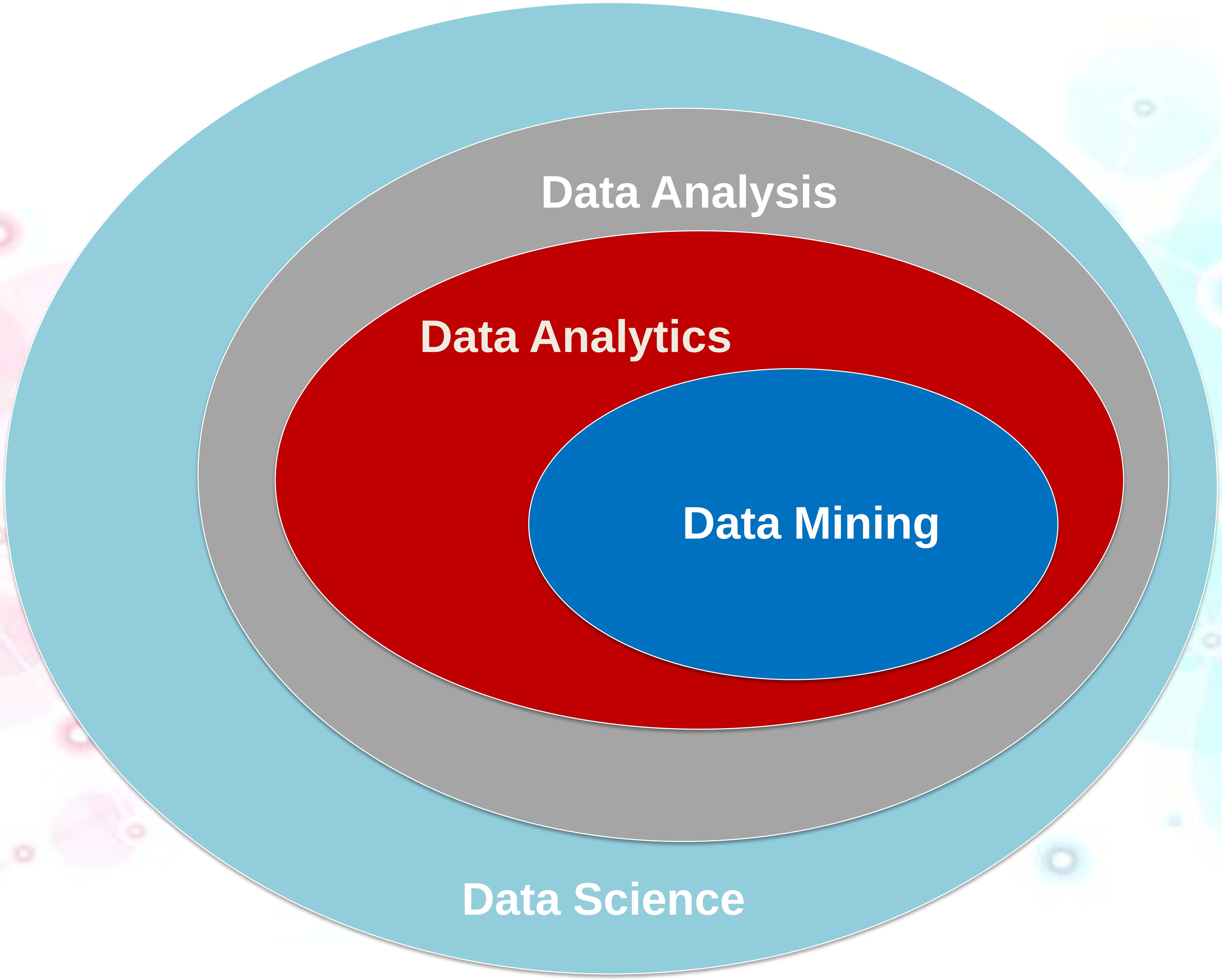
But the items are highly disordered:

In this case we will miss excellent mangoes. That is a keyword search used by all of us.

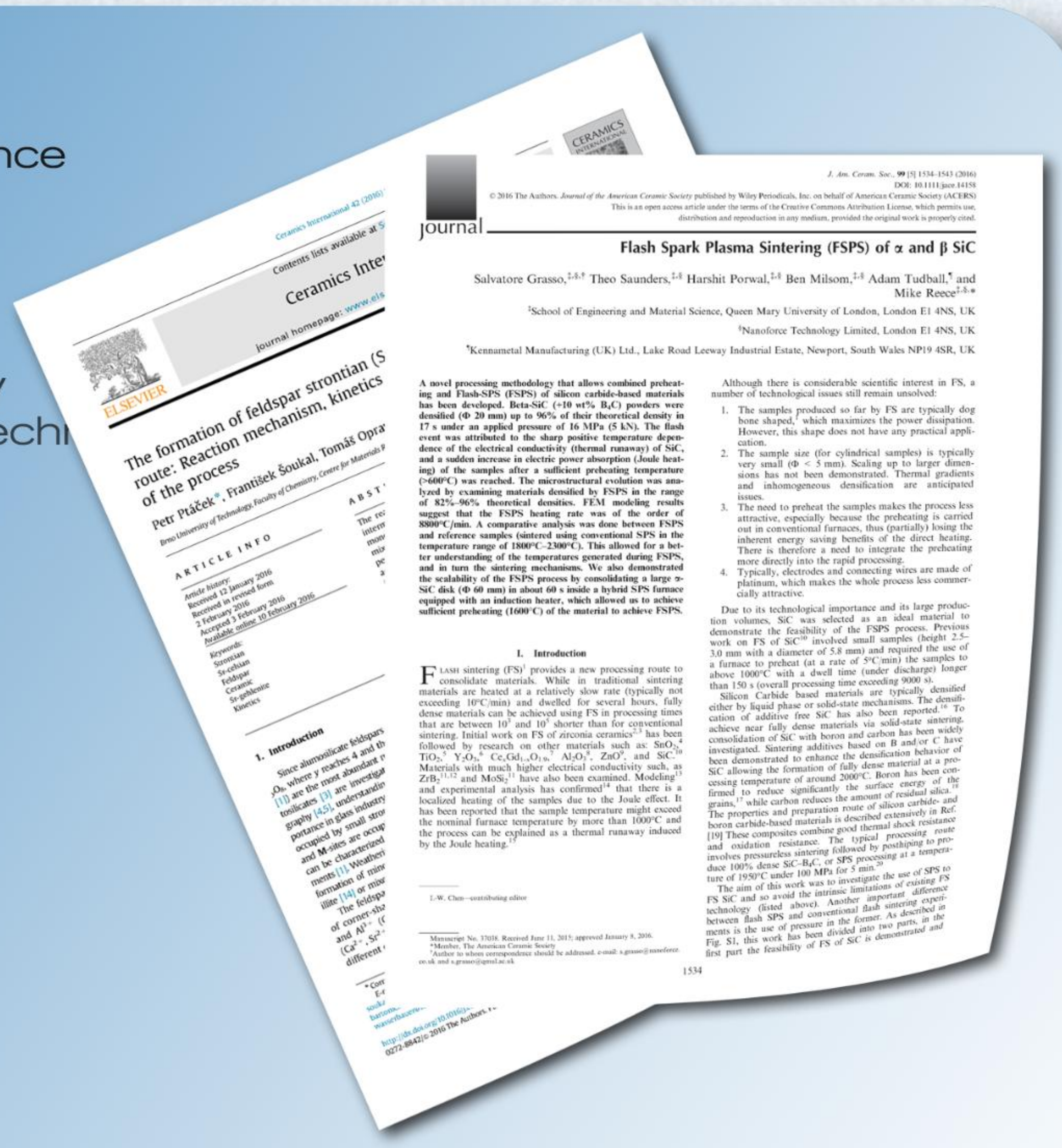
How could we overcome keyword search approach?

Using modern data processing approaches.

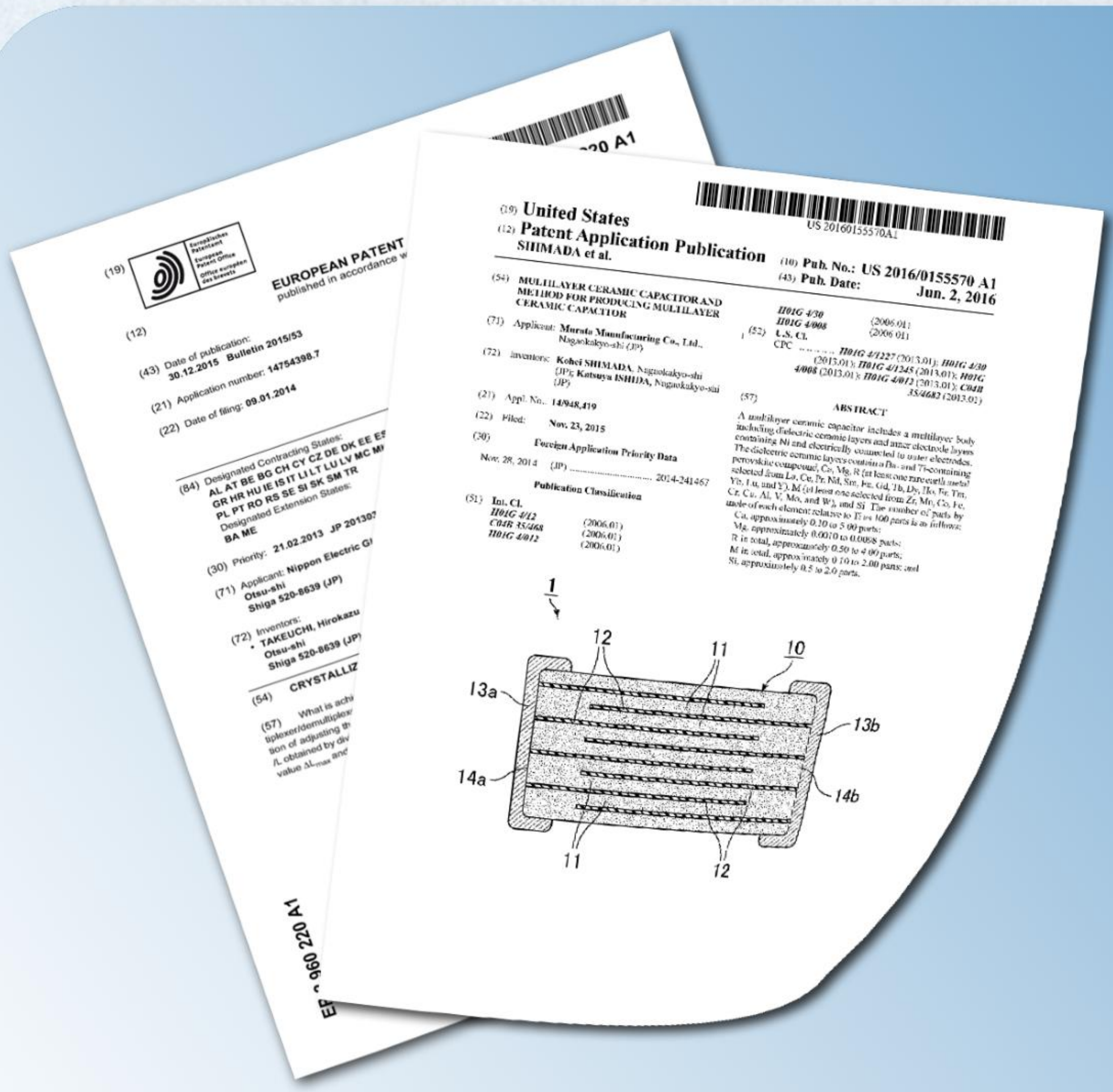
The core of all data techniques and tools is data mining



1. Journal of the European Ceramic Society
2. International Journal of Applied Glass Science
3. Journal of the American Ceramic Society
4. Ceramics International
5. Journal of Non-Crystalline Solids
6. Journal of Electroceramics
7. Journal of Sol-Gel Science and Technology
8. International Journal of Applied Ceramic Techn
9. Advances in Applied Ceramics
10. Acta Materialia
11. Journal of Alloys and Compounds
12. Journal of Solid State Chemistry
13. Materials Letters
14. Chemical Communications
15. Journal of Materials Chemistry A
16. Glass and Ceramics
17. Journal of Advanced Ceramics
18. Journal of Materials Science
19. Vacuum
20. Powder Metallurgy and Metal Ceramics
21. Journal of Solid State Chemistry
22. Journal of the Ceramic Society of Japan
23. Physics and Chemistry of Glasses
24. Journal of the Australian Ceramic Society



Journals



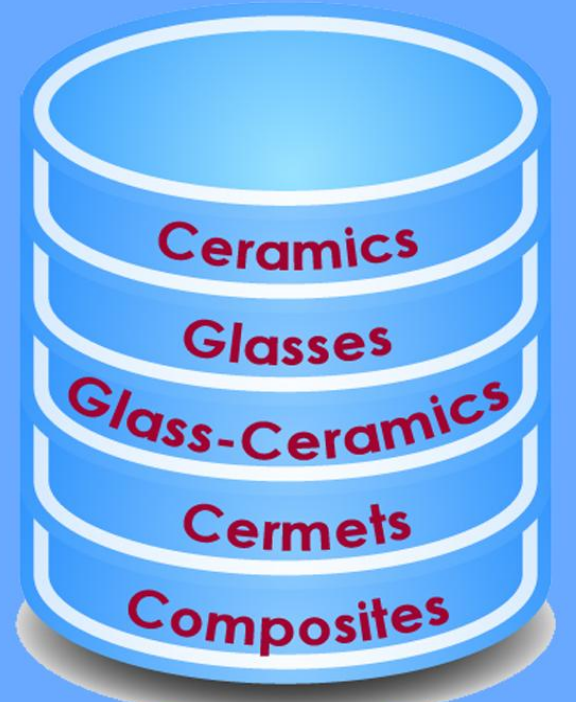
International Patent Classification Codes:

C03C

C04B { 33, 35, 38, 41/80, 41/85-91 }

Patent Applications

2 million data points!



GLACER Database

Near 100 types of numerical data

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The team of Natural Sciences Information Centre has key competence in data mining.

We had mined the experimental data on chemistry, nanotechnology, biotechnology, …

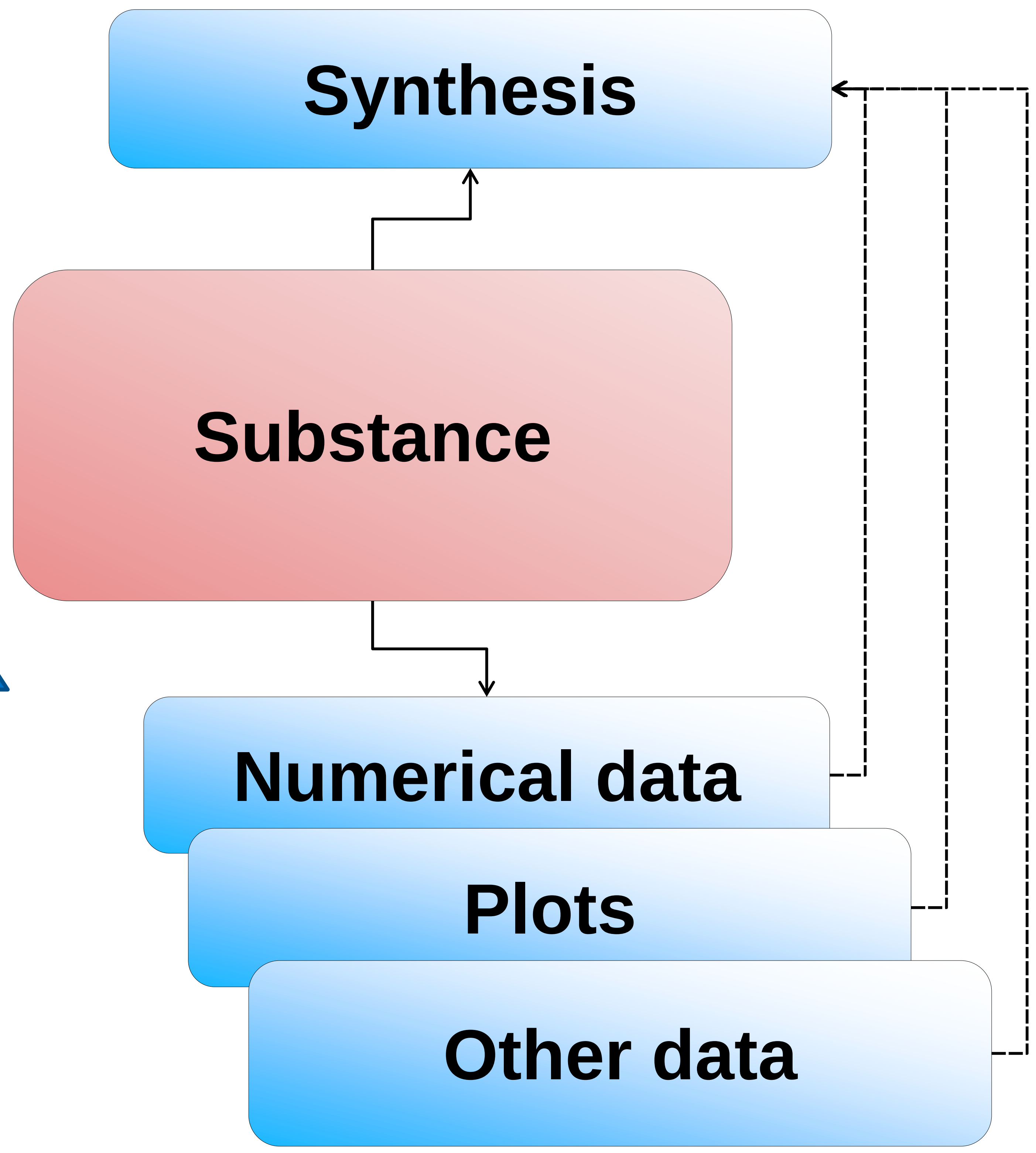
These branches of science now enjoy the structured data ready for analytics.

What about material science?

For many areas of material science the keyword search works not that bad. But not for graphical data in plots.

GlaCer database

Experimental data with preparation links



Articles and patents

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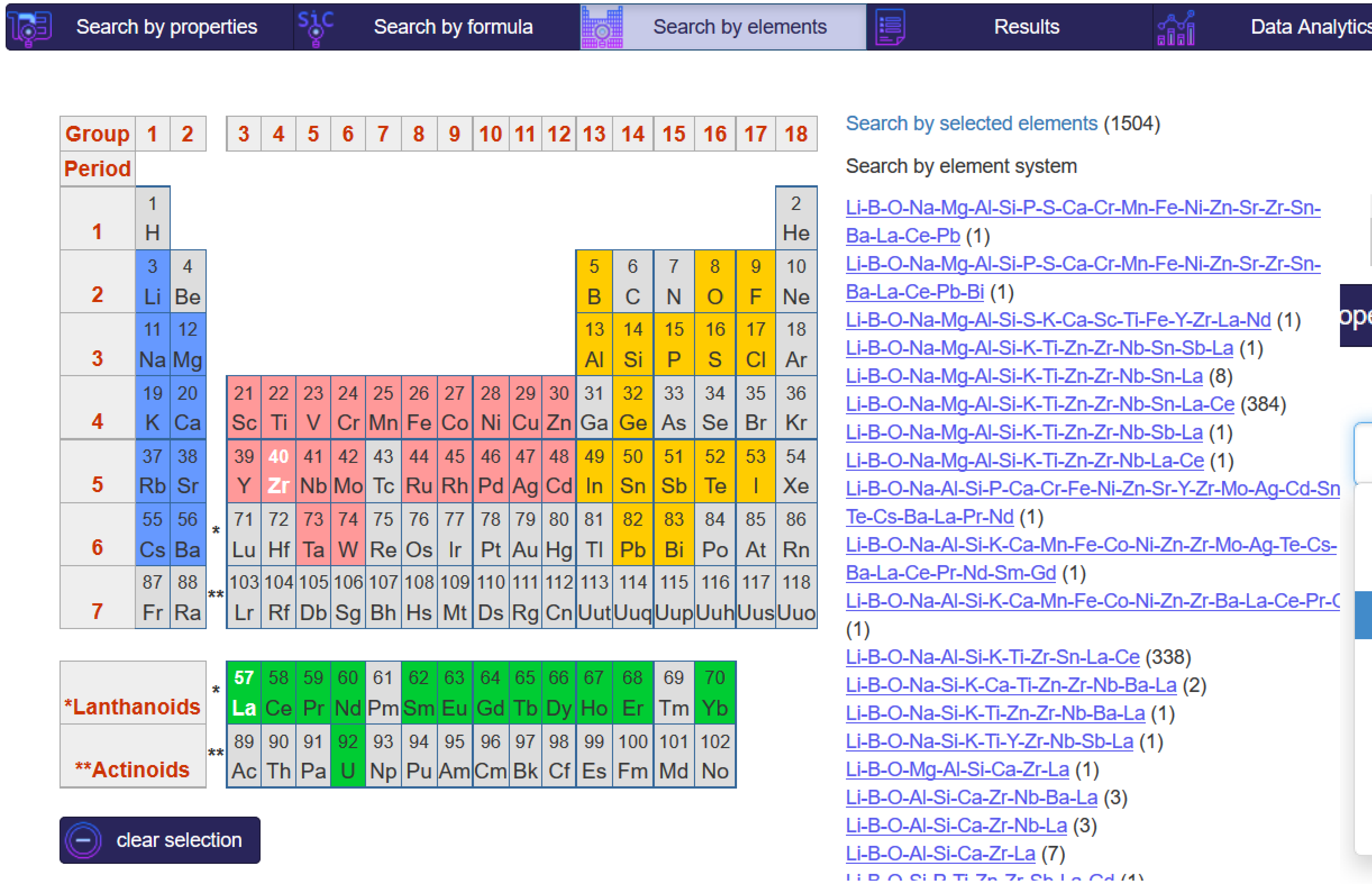
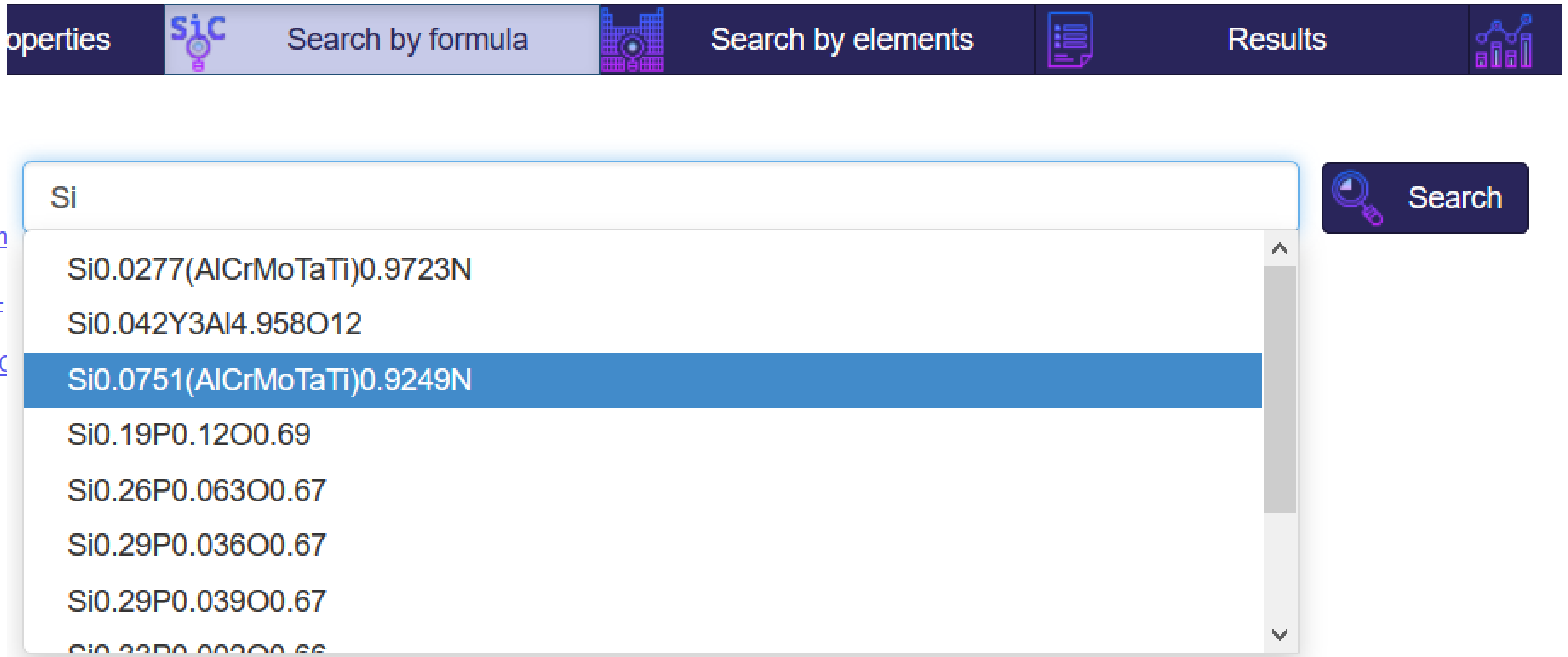
Easy search for materials

Search by elements



Search by formula



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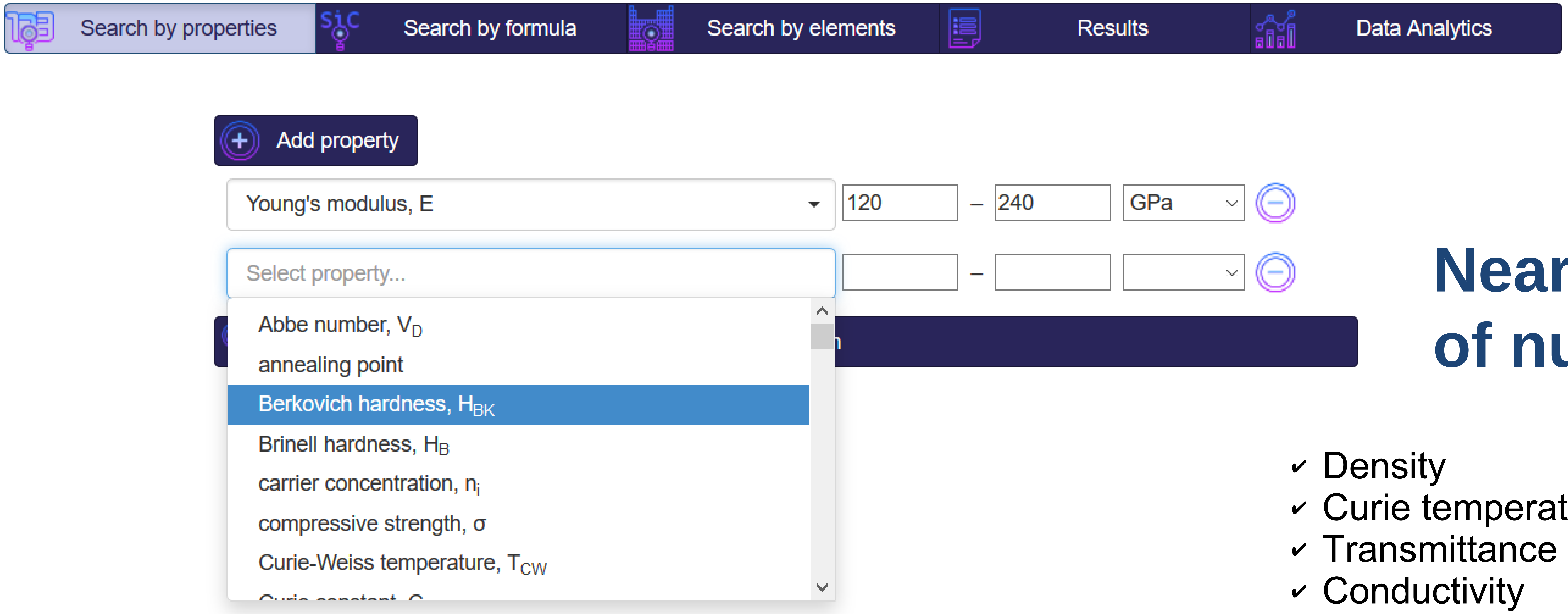
Search for required materials

Search by any combination of desired properties



Near hundred types of numerical data

- ✔ Density
- ✔ Curie temperature
- ✔ Transmittance
- ✔ Conductivity
- ✔ Piezo coefficients
- ✔ Permittivity
- ✔ Young's modulus
- ✔ Vickers hardness
- ✔ Flexural strength
- ✔ Loss tangent
- ✔ Thermal conductivity
- ✔ Dielectric strength
- ✔ Fracture toughness
- ✔ Compressive strength
- ✔ Wear coefficient
- ✔ Coercivity
- ✔ Remanence
- ✔ Poisson's ratio

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Graphical data plots

Original plot

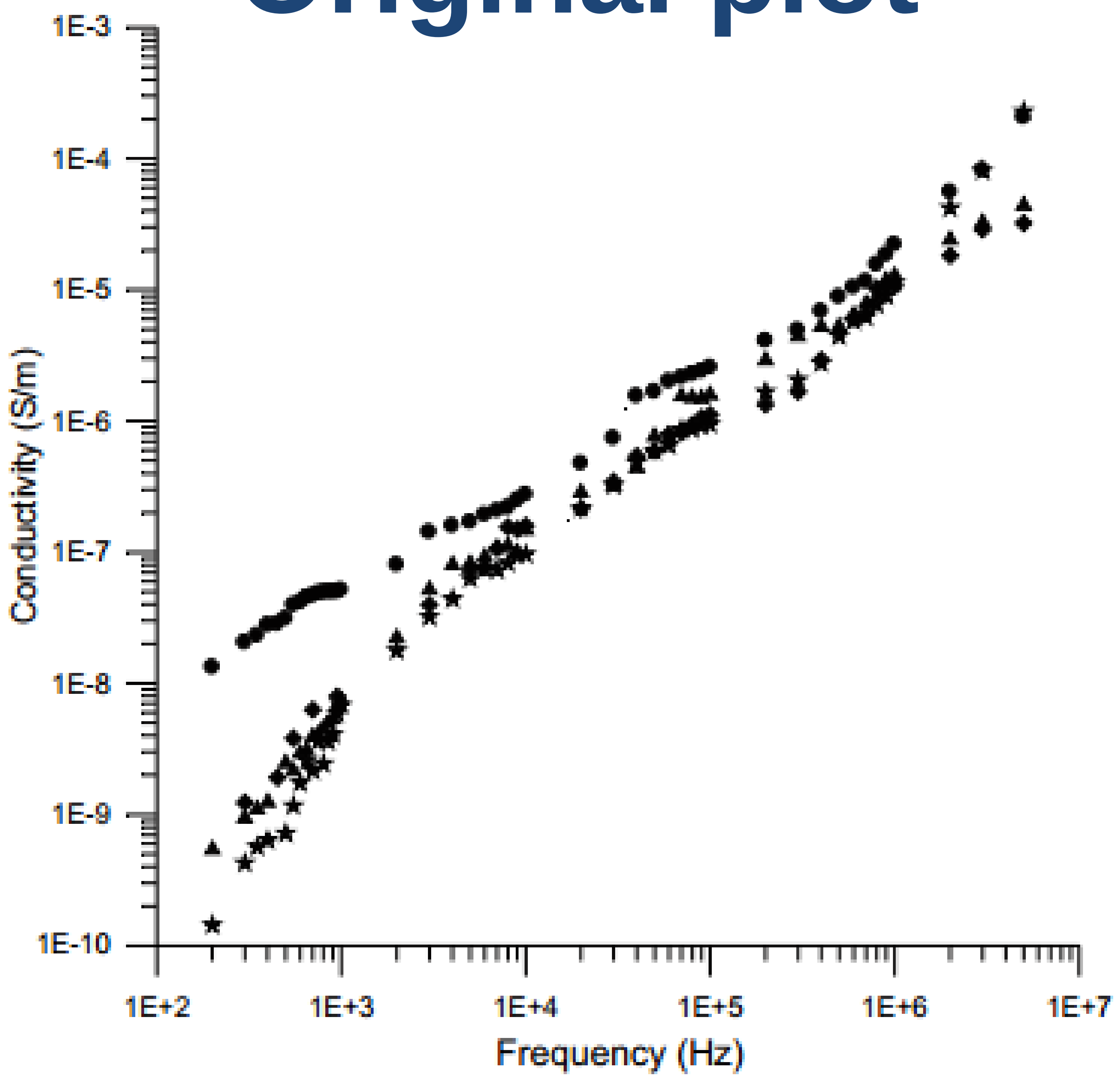
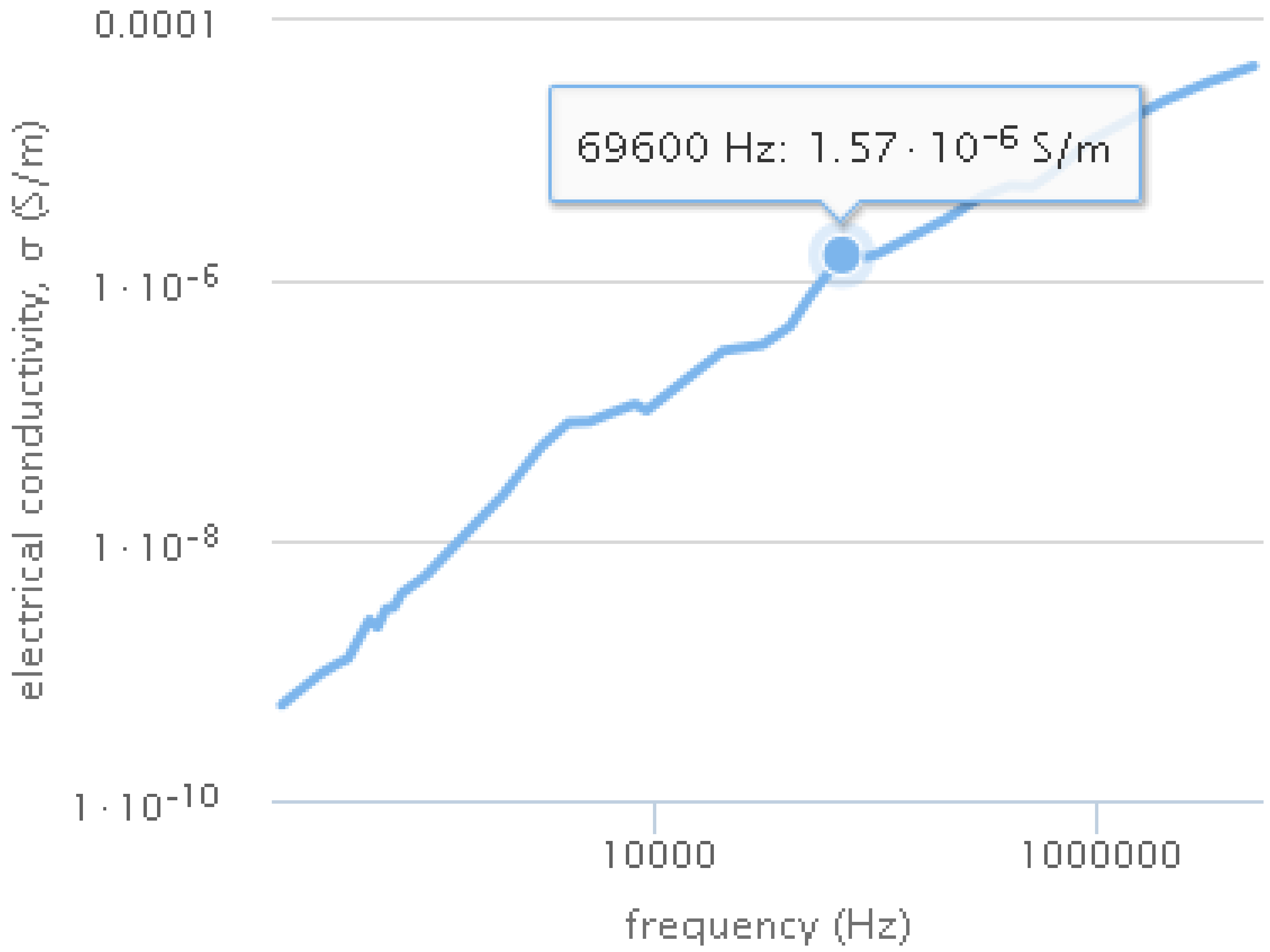


Fig. 5 Conductivity variation with frequency for samples G_1 (◆),G_2 (●), G_3 (▲) and G_4 (★).

Taken from
Ibrahim, S., Gomaa, M.M. & Darwish, H.
J Adv Ceram (2014) 3: 155

Values are searchable in database!

digitized interactive plot



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Even derived data are accessible by search

Example of derived data

Abstracted:

• Permittivity ε‘

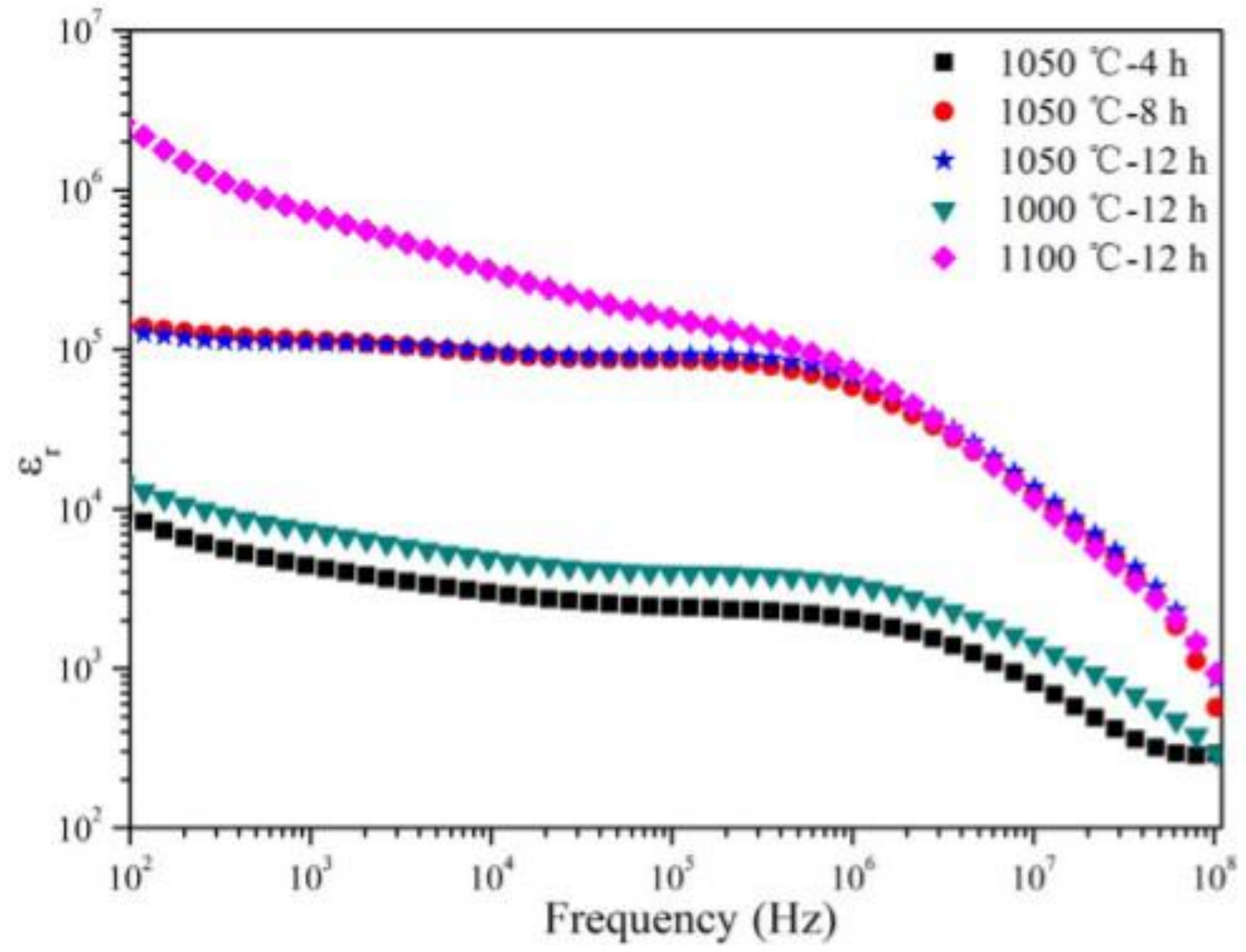
• Loss tangent tan δ

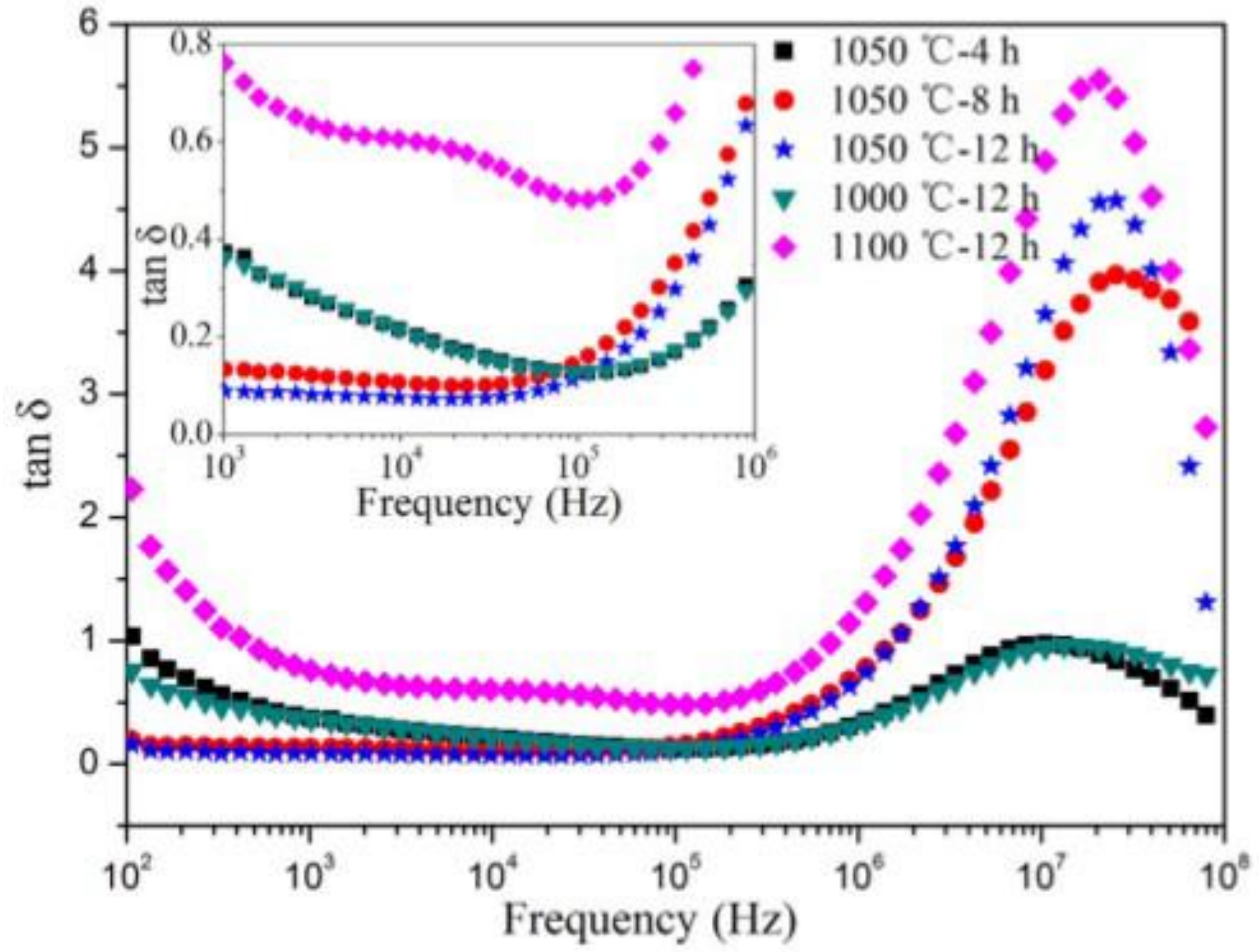
Auto

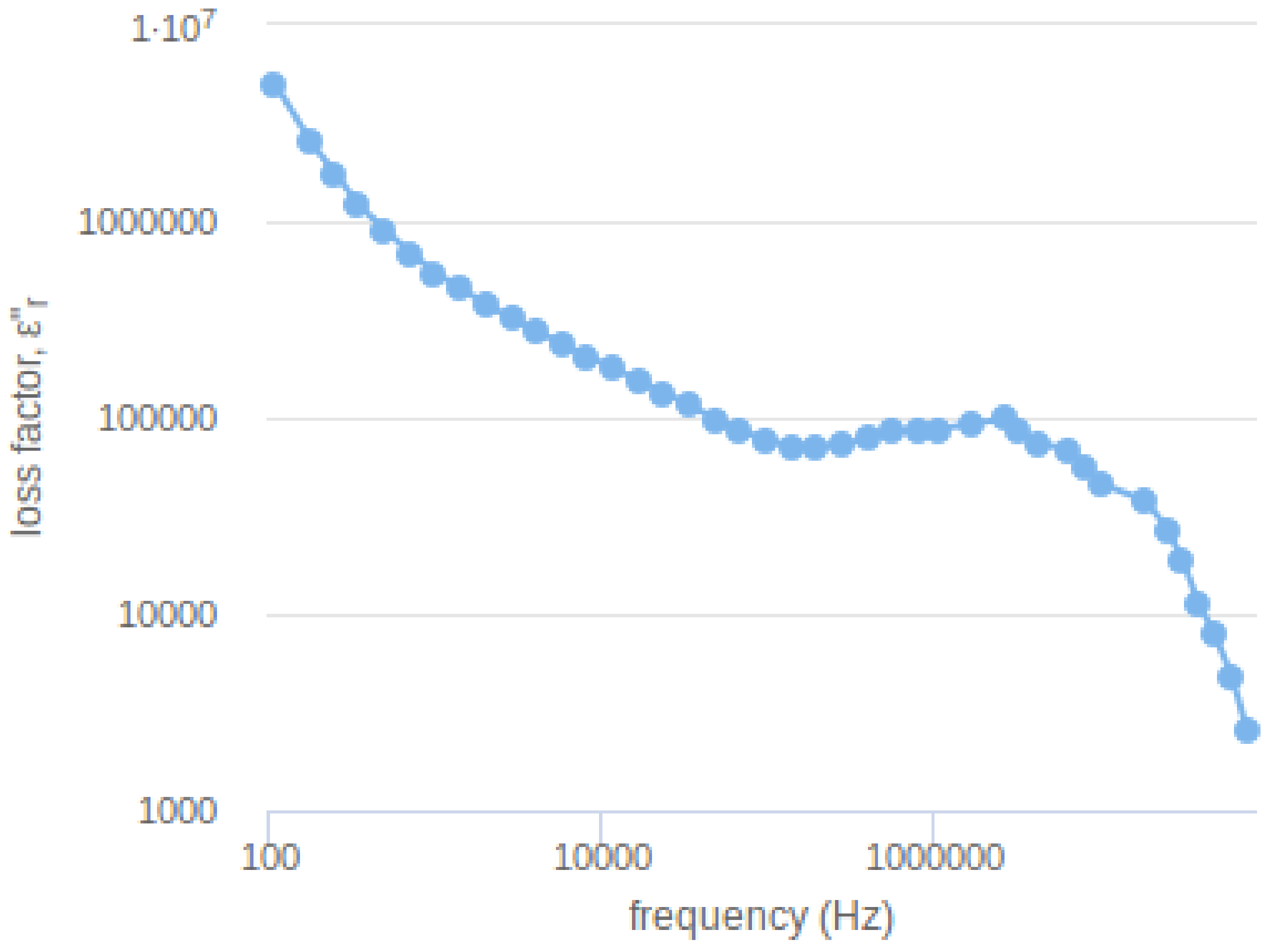
Converted to:

Loss factor ε''

(ε'' = ε' * tan δ)







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Derived numerical data

Definitions and laws of physics

TABLE 1

Exemplary Clad Glass Compositions

	1	2	3	4	5	6	7
SiO_2	30	25		8.3	8	7.72	7.46
Al_2O_3	15	15	34.6	33	31.79	30.67	29.62
B_2O_3							
MgO	5	5	3.8		3.66	3.53	3.41
CaO			61.6	58.7	56.55	54.55	52.69
SrO						3.53	3.41
ZnO	5	5					3.41
La_2O_3	10	15					
Ta_2O_5	30	30					
Y_2O_3	5	5					
ZrO_2							
Li_2O							
TiO_2							
Shear Modulus (GPa)	53.77	53.88	42.93	41.32	41.9	41.91	42.16
Young's Modulus (GPa)	141.62	142.42	109.7	105.68	107.39	107.06	108.07
Annealing Point (C.)					814.5	807	783.5
Strain Point (C.)					780.7	772.1	747.9
Softening Point (C.)	938.5				947.5	942.6	924.2

$$E=2\cdot G\cdot(1+\nu)$$

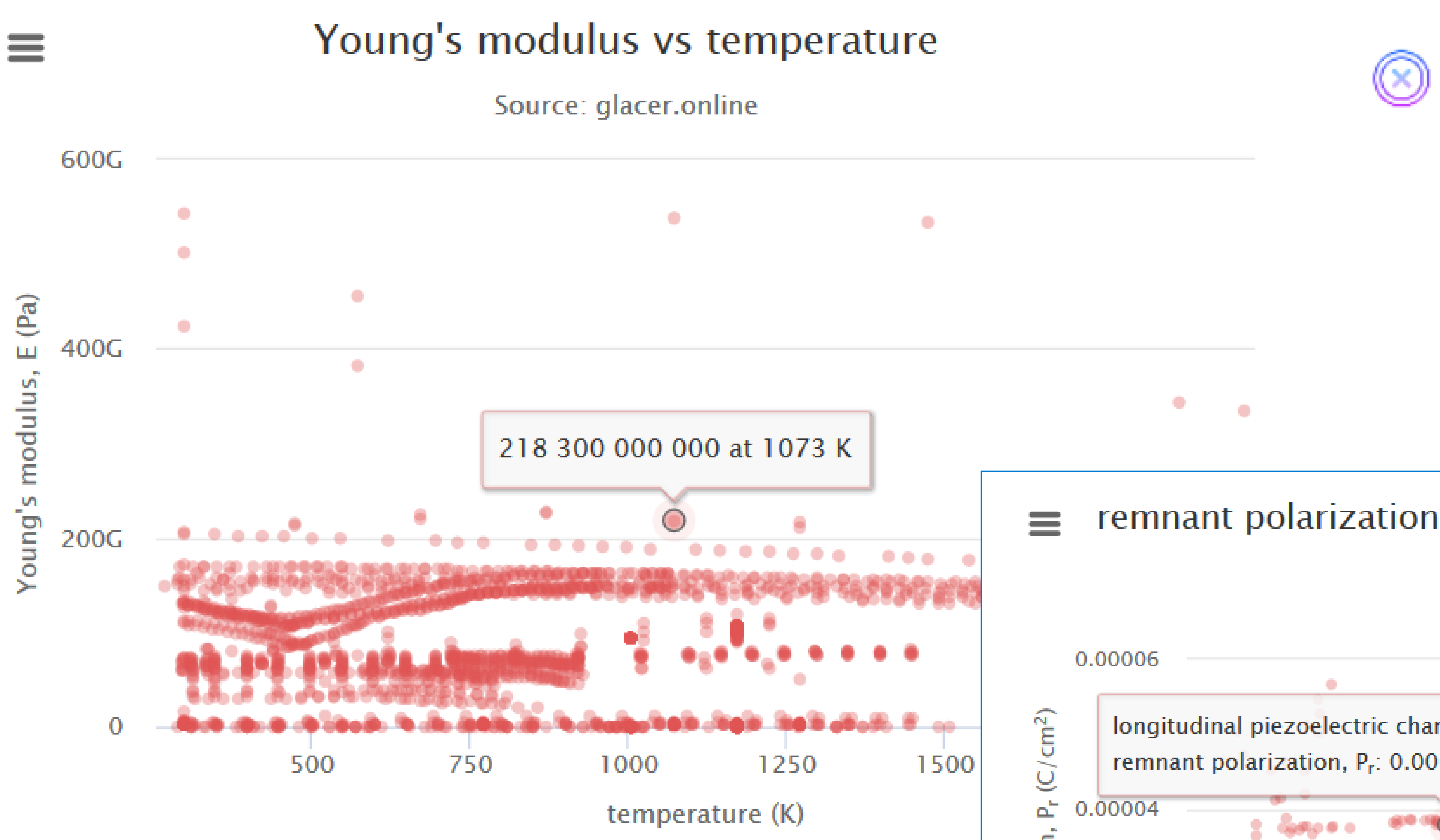
Glass	Poisson's Ratio
1	0,32
2	0,32
3	0,28
4	0,28
5	0,28
6	0,28
7	0,28

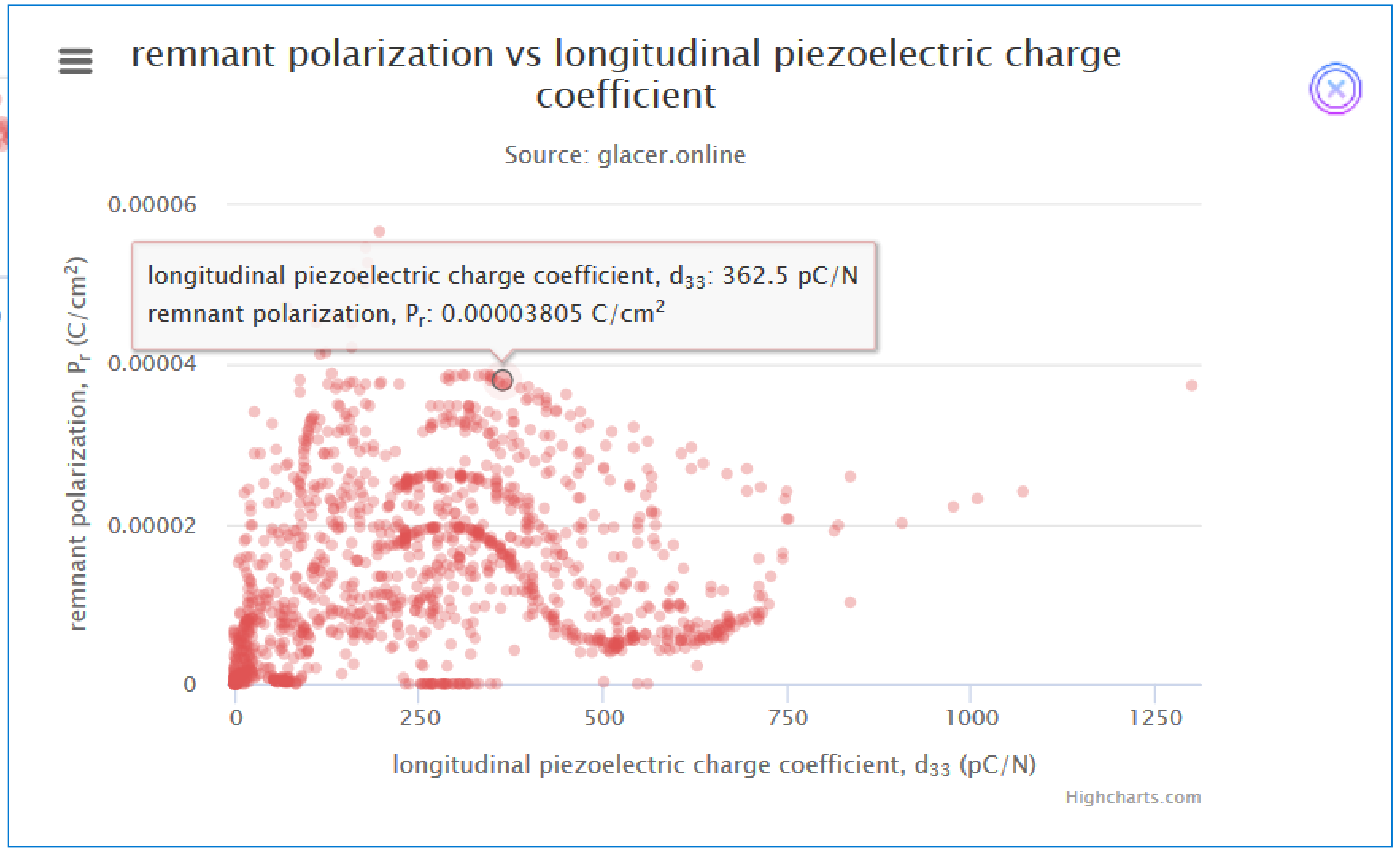
Data analytics

Useful correlations and statistics for search results

Search by properties | Search by formula | Search by elements | Results | Data Analytics

- **Boxplot**
- **Correlation**
- **Temperature distribution**
- **Parameter vs atom content**
- **Wordcloud**





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Search example

Transparent conductive films

- High transmittance (>80%)
- High electrical conductivity (>1000 S/cm)

- Solar panels
- Touch screens
- Smart windows

Search example

Telecommunication materials

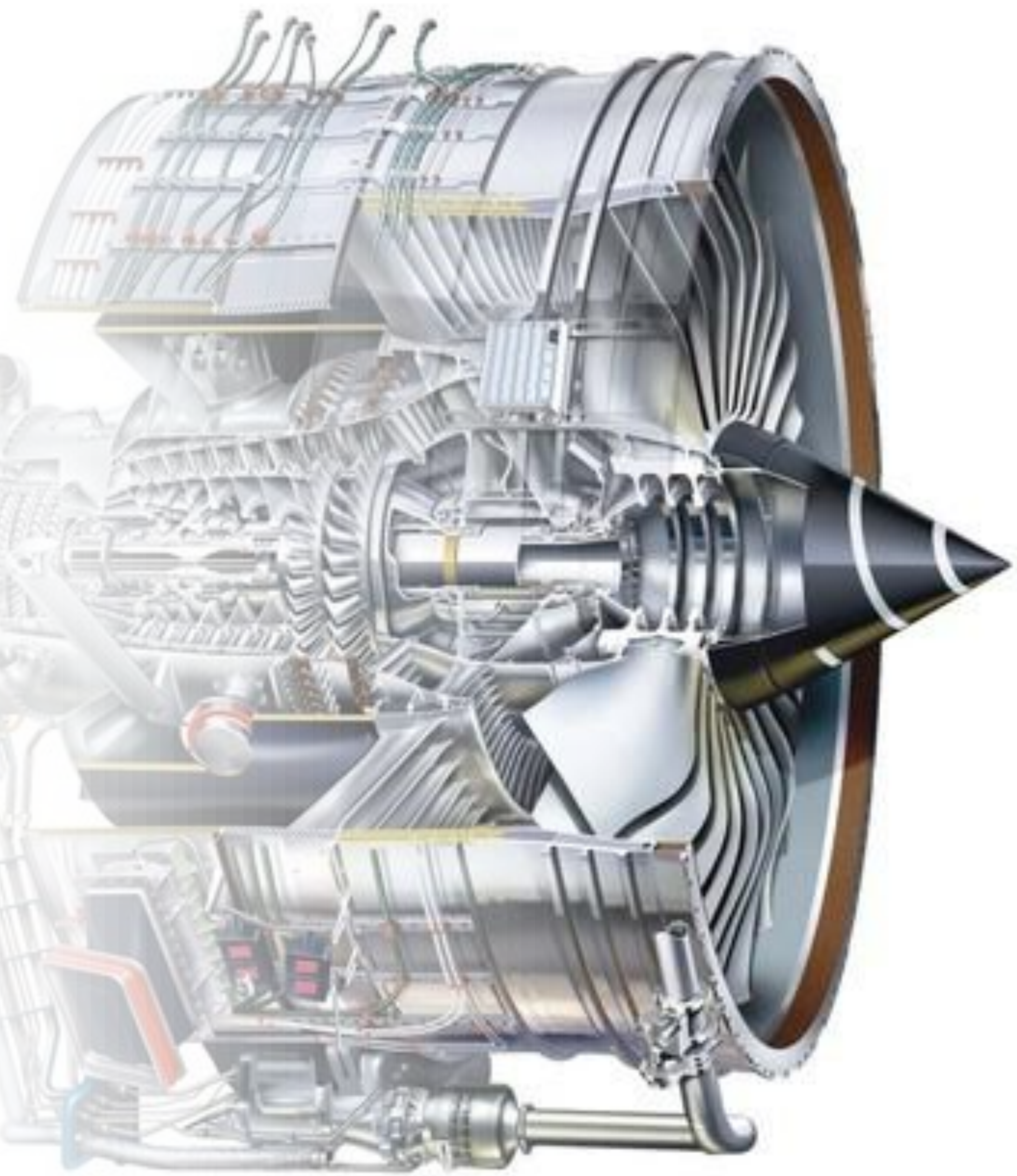
- High relative permittivity (> 10 000)
- At t = 80-100 °C
- In narrow frequency region (4.8-4.9 MHz)

Search example

Thermal barrier coatings

- Low thermal conductivity (< 2 W/m*K)
- Linear expansion coefficient (1-10 ppm/K)
- No rare earth elements

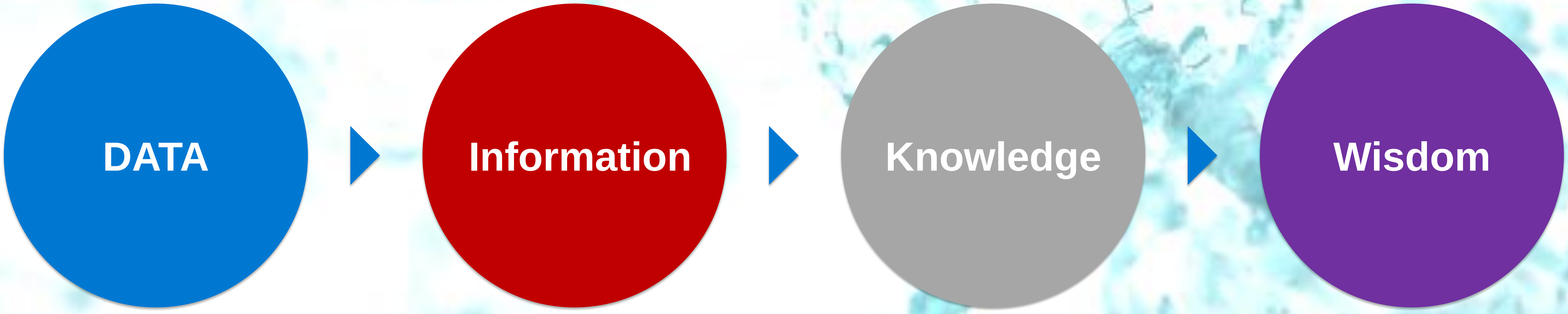
- Turbine blades
- Combustion chambers



Extreme properties

Wonderful materials

- Fe:BN core-shell metamaterial: **ε'_r = − 100 000** at 23 MHz
- Nanofibrous YSZ: **E** = **0.016** GPa
- TiB_2 + 2.5 wt% EuB_6: **E** = **659** GPa
- Foam-like hexagonal boron nitride: **ρ** = **0.0017** g/cm^3
- $Mn_3Cu_{0.9}Si_{0.1}N$: **CTE = − $6.3 \cdot 10^{-6}$** °C^{-1}


DATA
Information
Knowledge
Wisdom

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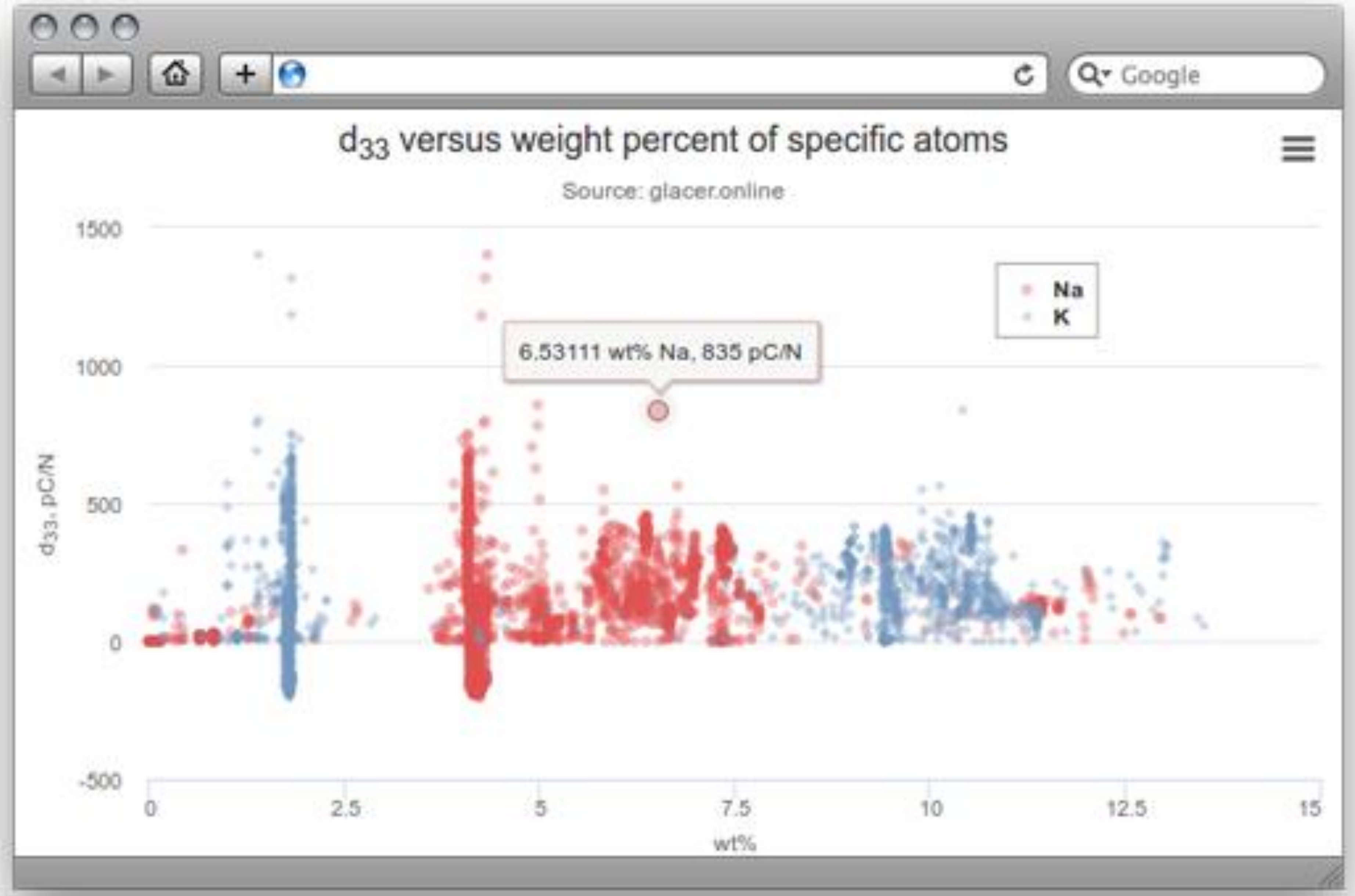

Property	Value	Parameters	Details	Preparation reference	Citation
dielectric strength, E_b	14 kV/mm				Ootomo, M. *et al.* (2015)
dielectric strength, E_b	35.9 kV/mm	thickness 1 mm	rectified AC	preparation 4	Neusel, C. *et al.* (2015)
dielectric strength, E_b	83.2 kV/mm	thickness 0.36 mm	DC	preparation 4	Neusel, C. *et al.* (2015)
dielectric strength, E_b	55.6 kV/mm	thickness 1.03 mm	DC	preparation 4	Neusel, C. *et al.* (2015)
electrical resistivity, ρ	$2.45 \cdot 10^{15}$ Ω·cm				Su, G.-Q. *et al.* (2014)
flexural strength, σ	325 MPa			preparation 9	Li, D. *et al.* (2016)
flexural strength, σ	350 MPa				Schneider, J. *et al.* (2016)
flexural strength, σ	477 MPa			preparation 4	Neusel, C. *et al.* (2015)
fracture toughness, K_{Ic}	3.7 MPa·m$^{1/2}$				Schneider, J. *et al.* (2016)
fracture toughness, K_{Ic}	2.7 MPa·m$^{1/2}$	load 20 N		preparation 7	Fedosova, N.A. *et al.* (2015)