NOMAD

NOVEL MATERIALS DISCOVERY

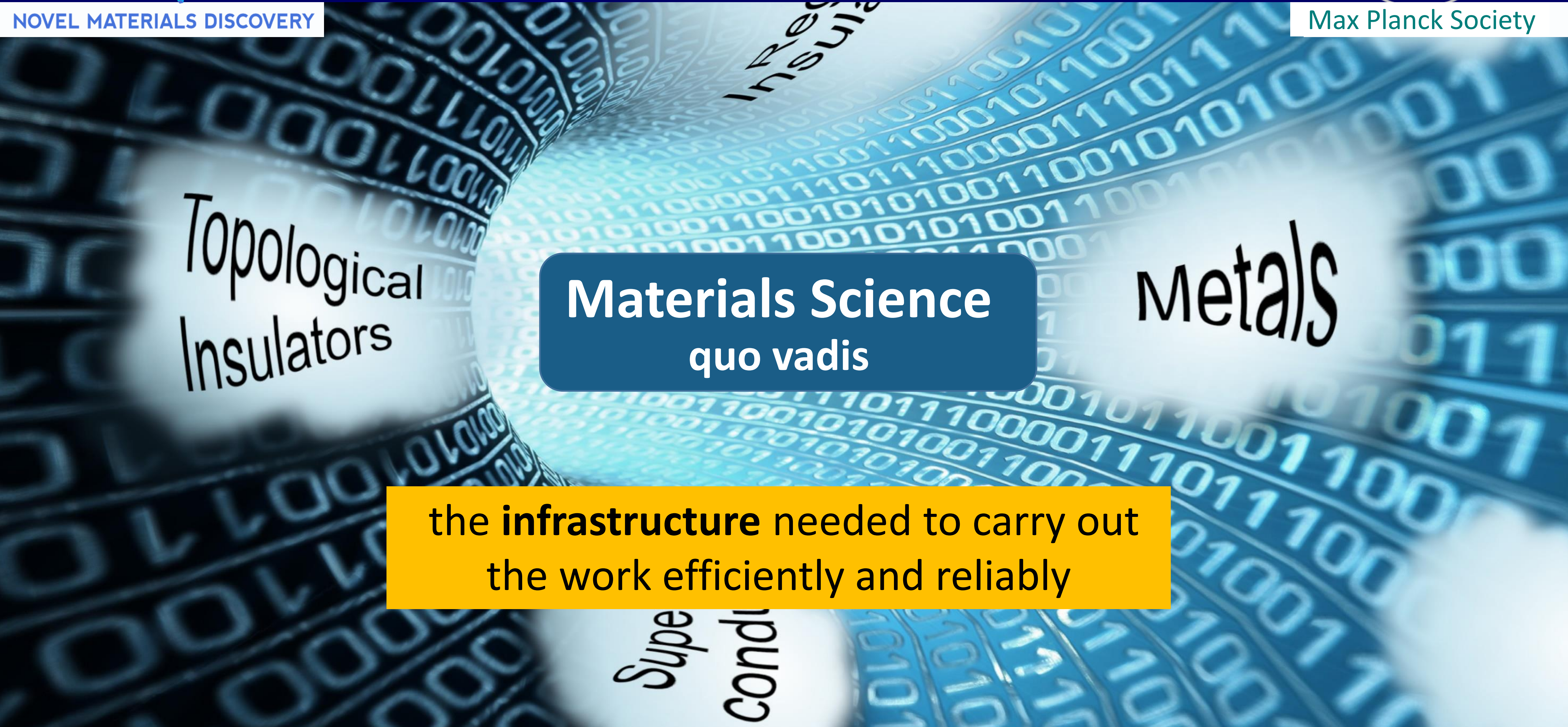
Perspectives in Materials Science

Max Planck Society

Materials Science
quo vadis

Big-Data Driven Materials Science
(The 4th Paradigm of Materials Research)

Perspectives in Materials Science



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the **infrastructure** needed to carry out the work efficiently and reliably

High-Throughput Screening in Computational (and Experimental) Materials Science

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Consider as many compounds a possible, typically $O(10^3)$ – $O(10^5)$

Sharing Advances Science

Needs for a FAIR, Efficient Research-Data Infrastructure

Recycle the “waste”! Enable re-purposing.

$O(10^1)$ compounds selected

Animation by G.-M. Rignanese

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Findable Accessible Interoperable Reusable

M. D. Wilkinson et al., Scientific Data **3**, 160018 (2016)

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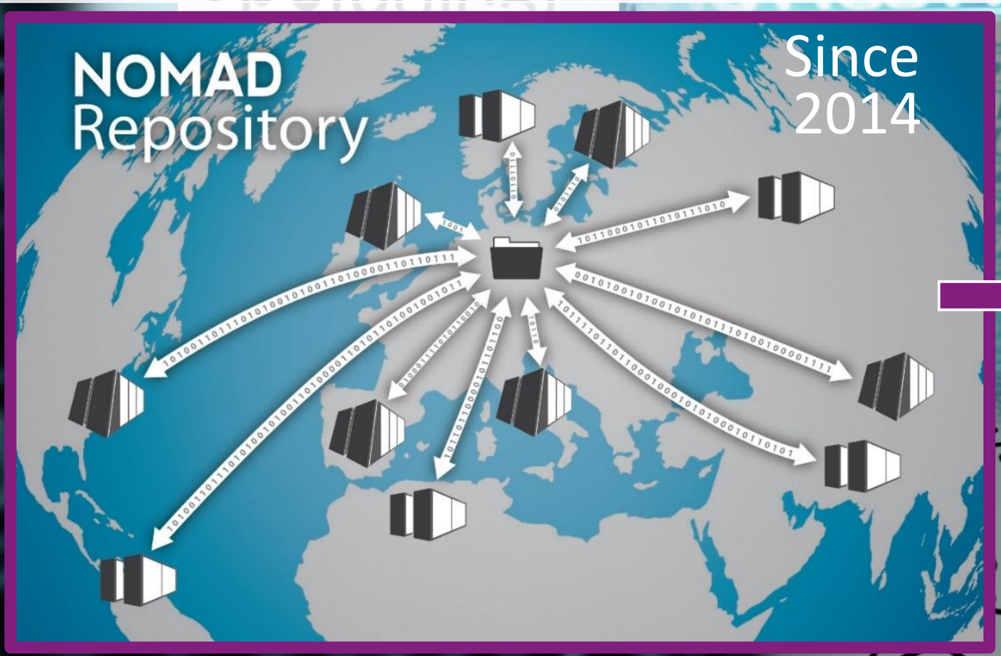
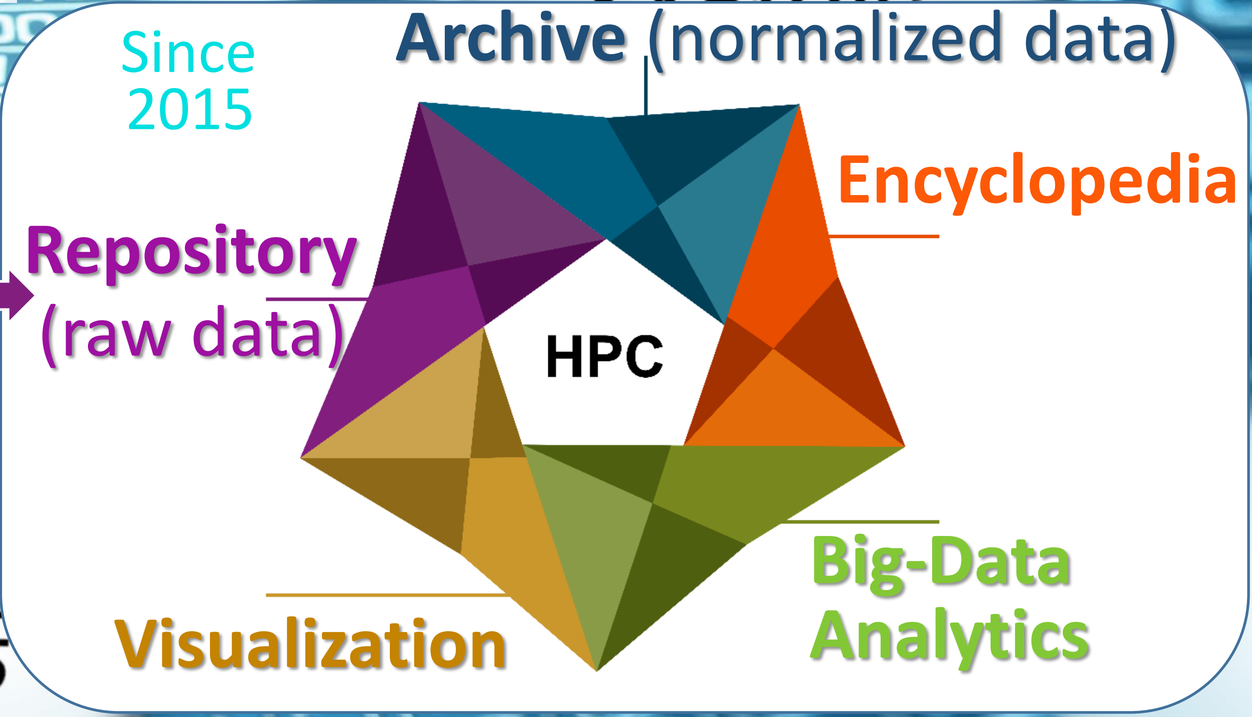
Requests the full input and output files



The NOMAD Center of Excellence



The NOMAD Repository
>100 Mio. DFT Calculations

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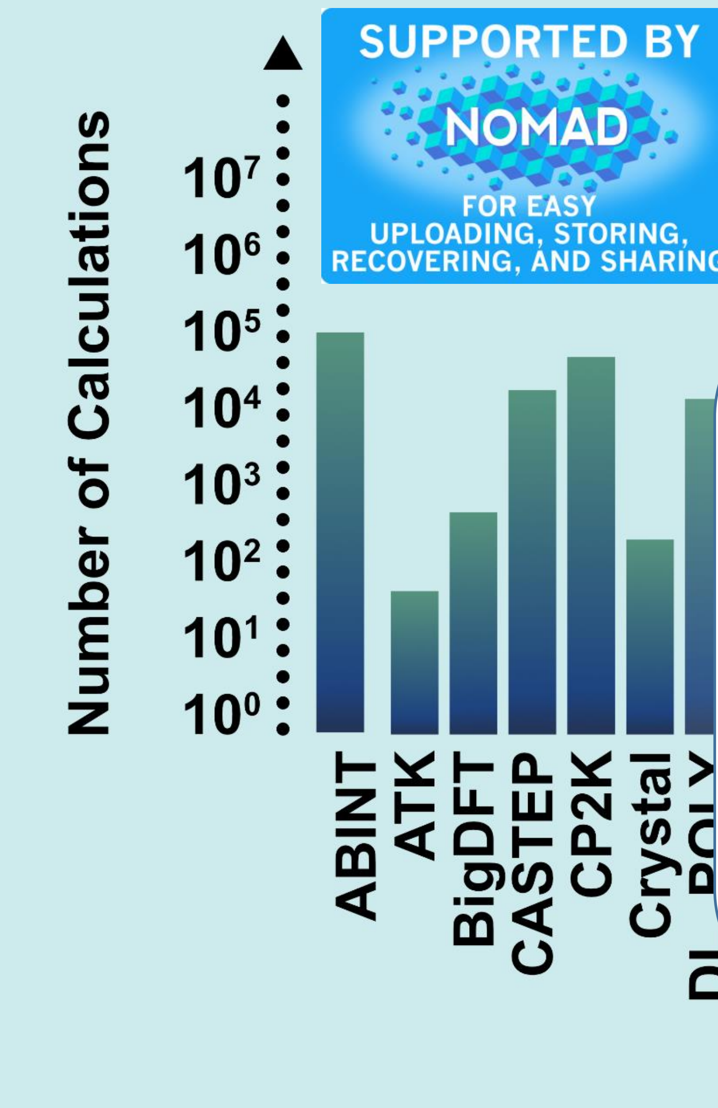

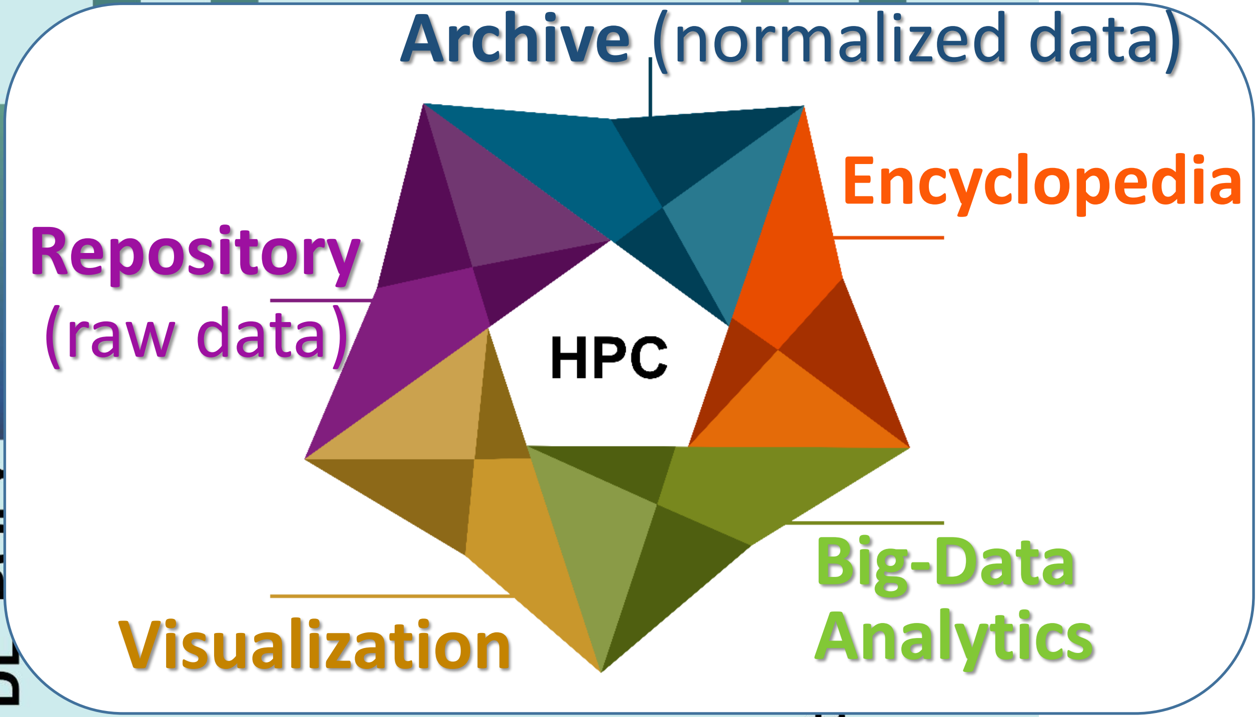

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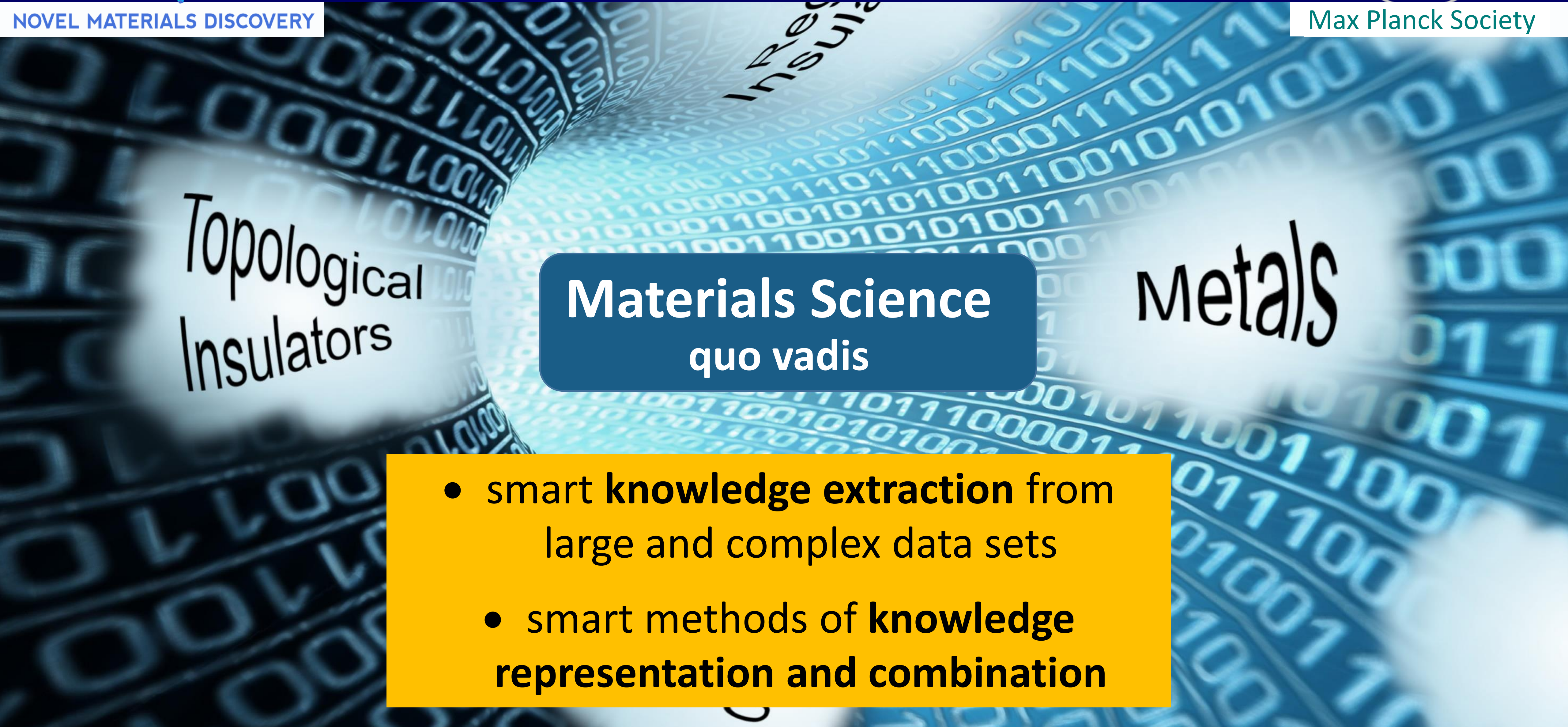

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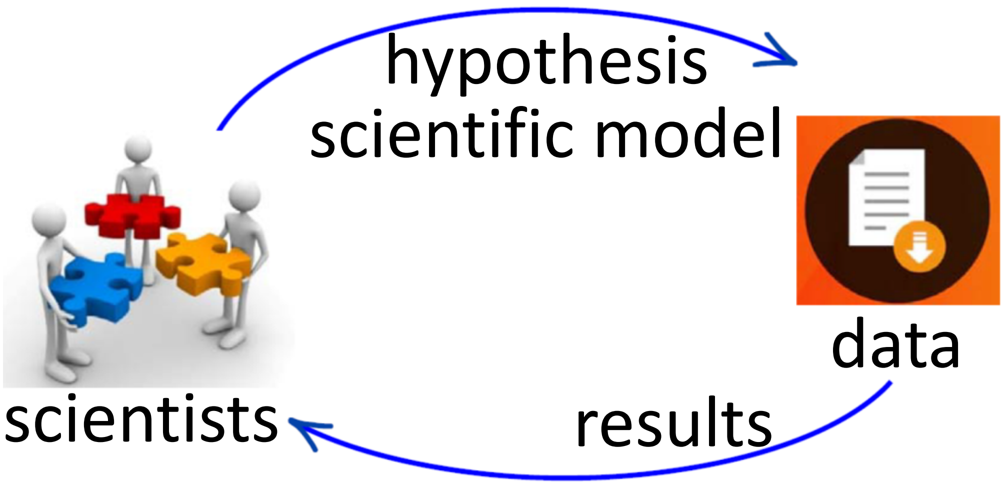
- smart **knowledge extraction** from large and complex data sets
- smart methods of **knowledge representation and combination**

“Maps of Materials Properties”

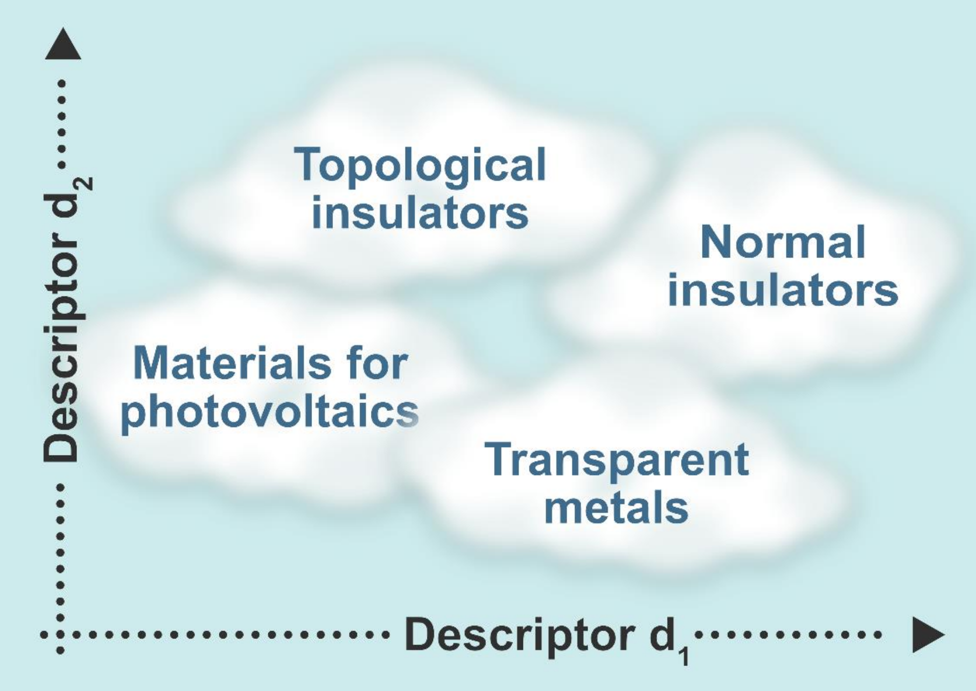
Adaptivity in science and data analysis

question



Feedback loop defeats
all available statistics

Building a “map of materials properties” from data, without a scientific model



Building "Maps of Materials Properties"
(Role Models: Periodic Table, Ashby Plots)

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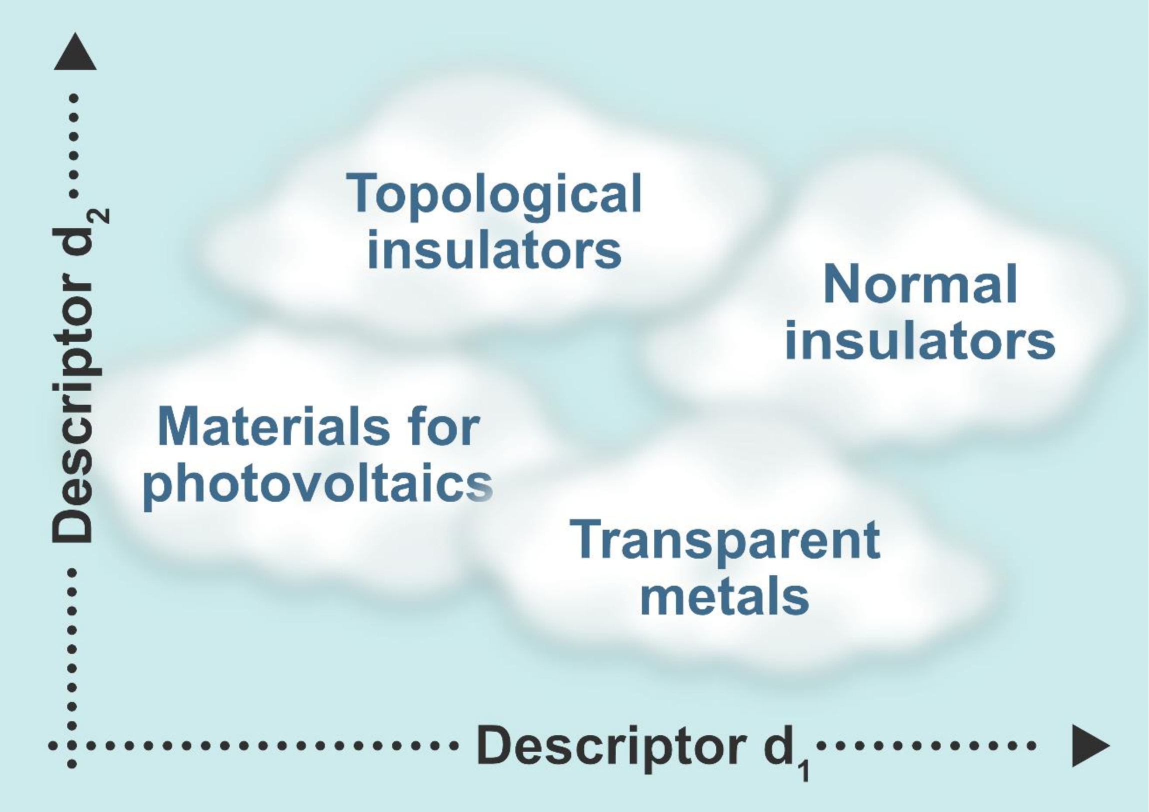

The science is in the determination (and understanding) of the descriptors. How to find them by statistical learning?

"Invert" the big-data problem:

Construct billions of *possible* descriptors and evaluate their values for N materials.

Find the strongest correlations of these N billion data points with computed (or experimental) results (properties) of the N studied materials. – *Sure Independent Screening and Sparsifying Operator (SISSO) by Ouyang, Ghiringhelli et al. (2018).*

Building Maps of Materials

(Role Models: Periodic Table, Ashby Plots)

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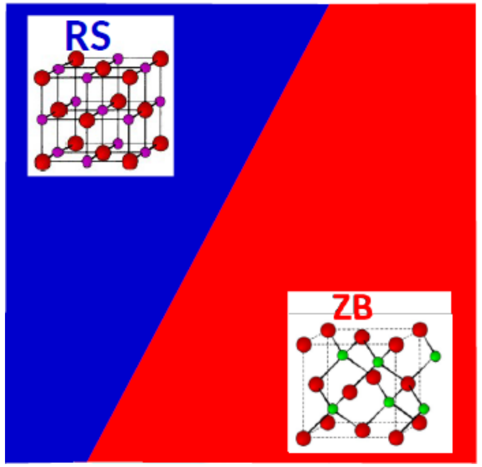
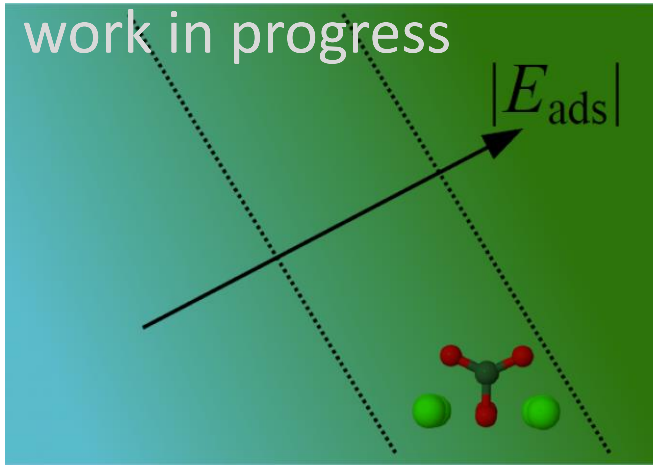
Crystal-structure prediction

- Octet binaries (ZB vs. RS)
- $Al_xGa_yIn_zO_3$ ($x+y+z=2$)
- Perovskites (Goldschmidt tolerance factor)

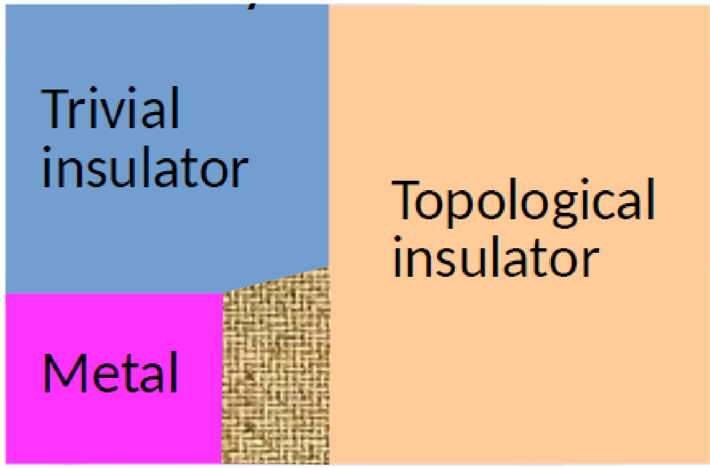


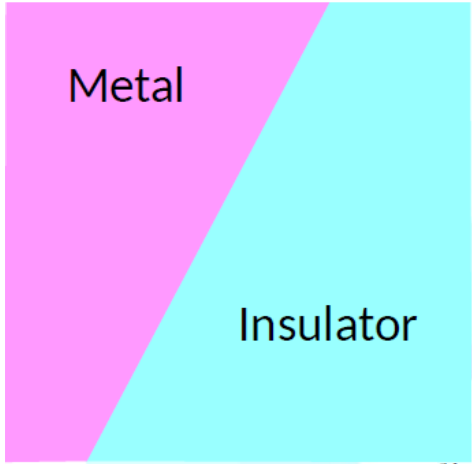


Activation of CO_2 at metal oxides and carbides

Property classification:

- Topological insulators



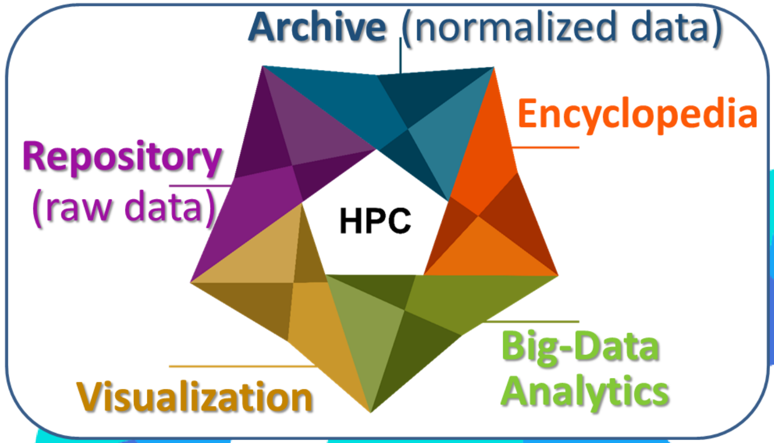


Property classification:

- Metal vs. insulator

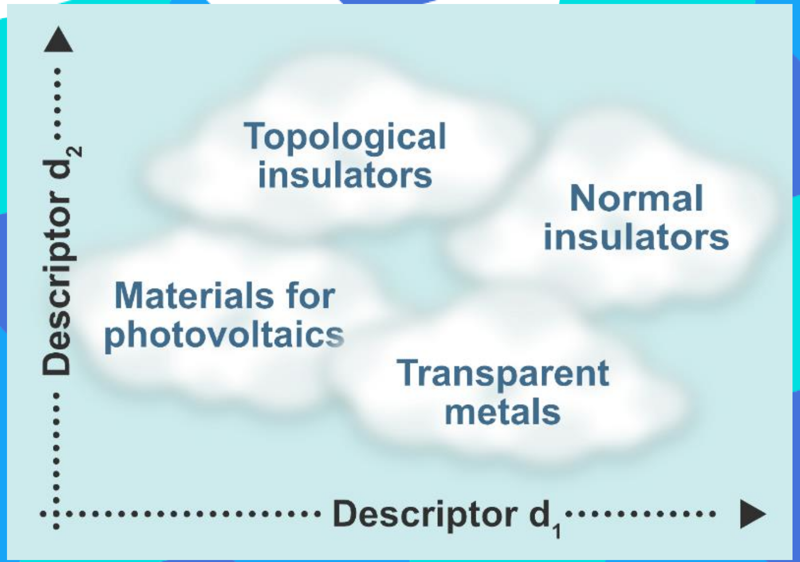
The Materials-Science Challenge Is Different to That of Standard Machine Learning

The **infrastructure** needed to carry out the work efficiently and reliably



Smart **knowledge extraction** from large and complex data sets

Smart methods of **knowledge representation and combination**



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Next Steps

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FAIR-DI

FAIR Data Infrastructure for Physics, Chemistry, Materials Science, and Astronomy e.V.

https://www.fair-di.eu

For a **F**ederated, **AI**–**R**eady DI

Video Conference on a
FAIR Data Infrastructure for Materials Genomics
(3-5 June, 2020)
A fantastic line-up of speakers

We need

- a federated system for data, as data are getting too large for been transported
- new (different) AI tools: domain specific AI; outlier detection, local vs. global models; bring codes to (federated/ distributed) data
- "complete" characterization of the measurement conditions by metadata (basis for reproducibility)
- to avoid (much) more load on the researcher (make metadata assignment and data standards automatic)
- IT and practical AI specialists