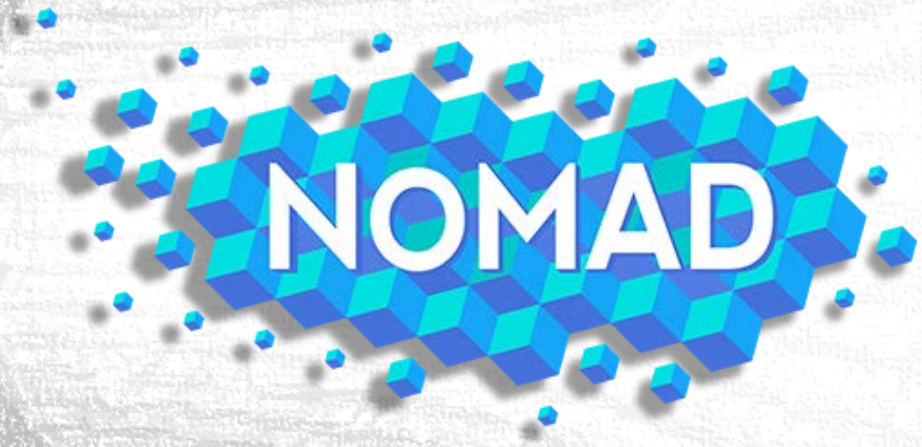
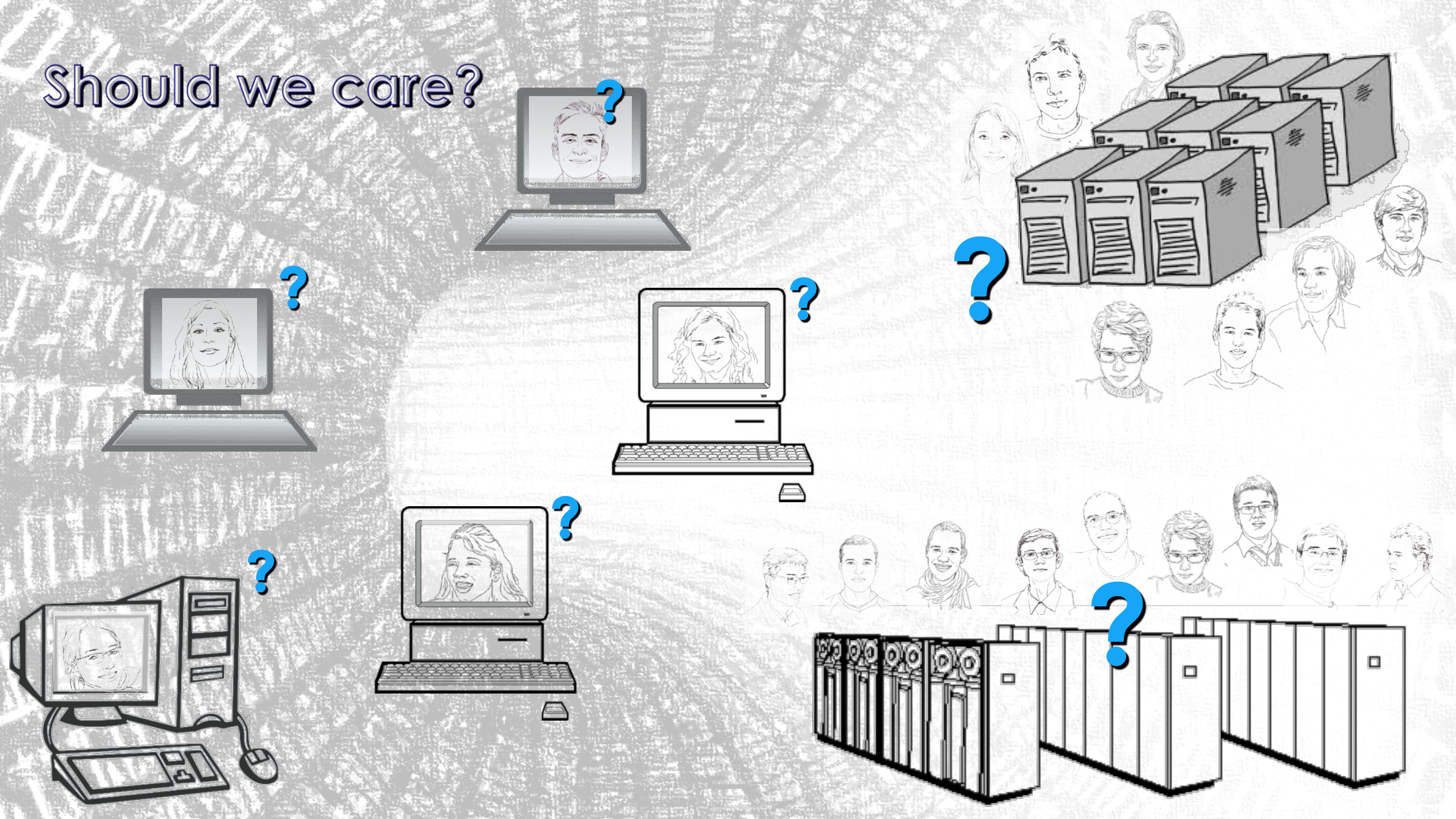


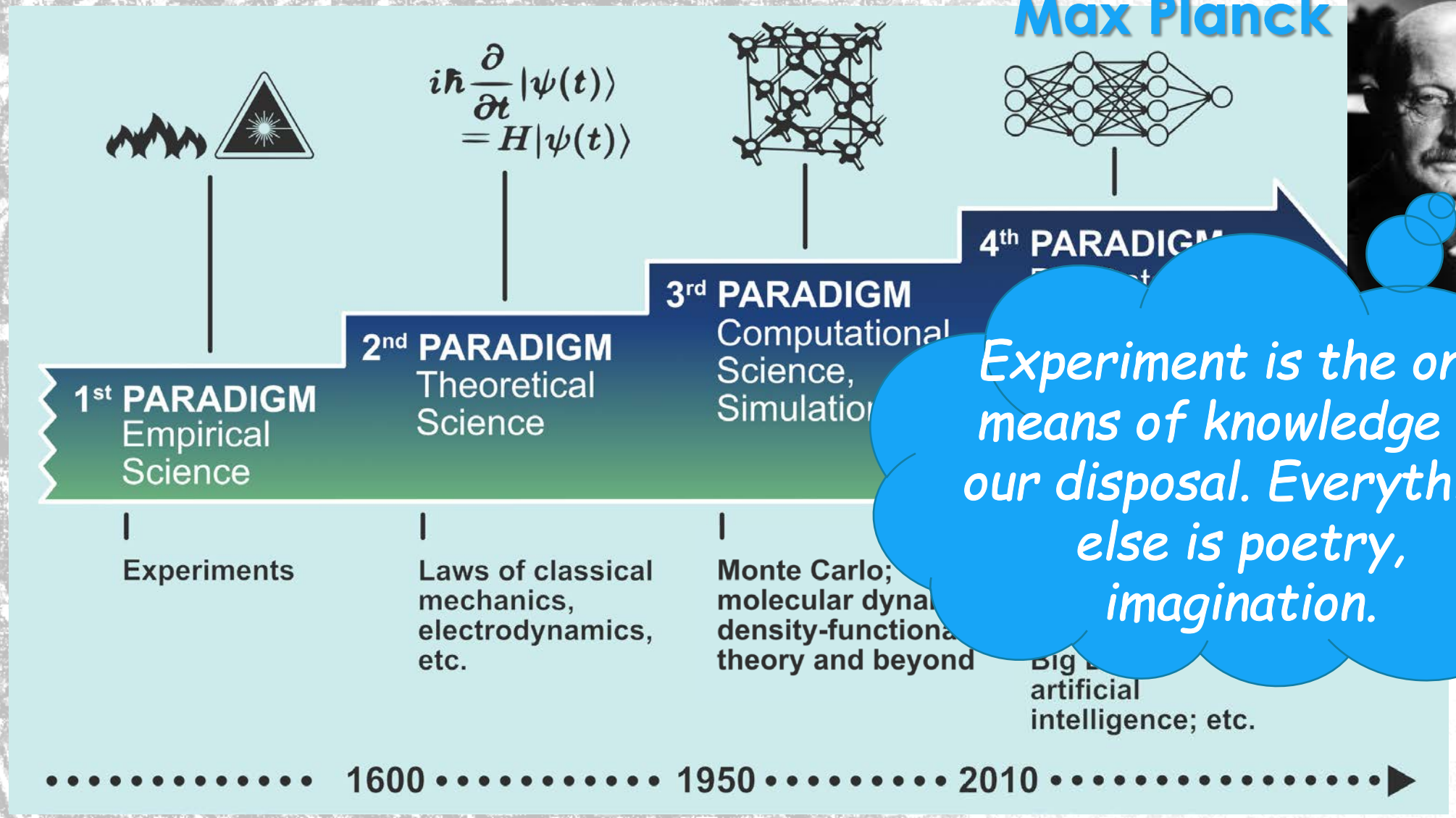
Claudia Draxl

Should we care?

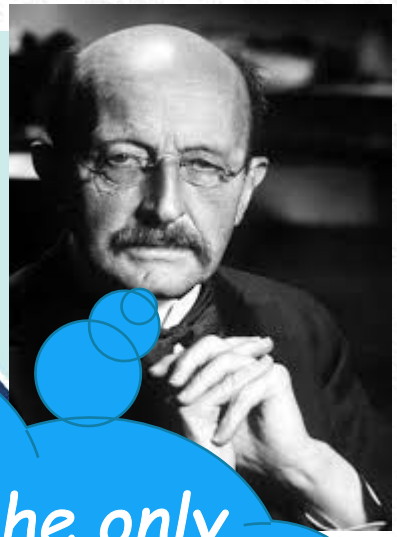


MRS MATERIALS RESEARCH SOCIETY®

From history to future ...



Max Planck

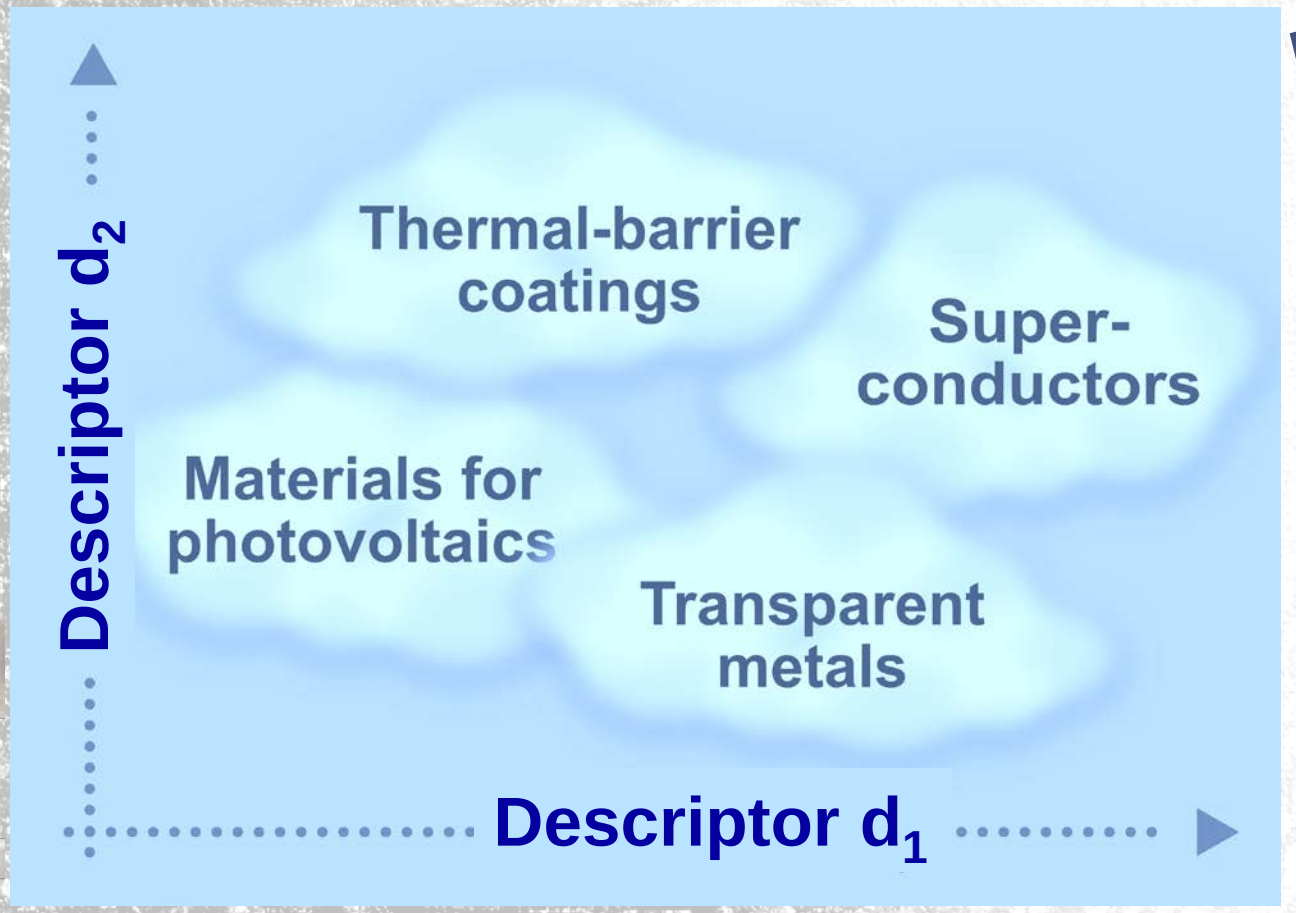


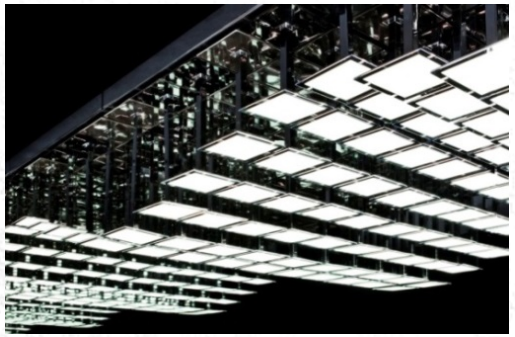
Experiment is the only means of knowledge at our disposal. Everything else is poetry, imagination.

Jim Gray (Jan. 11. 2007): The 4th Paradigm, Data Intensive Discovery, edited by Hey, Tansley, and Tolle

Our scientific vision …

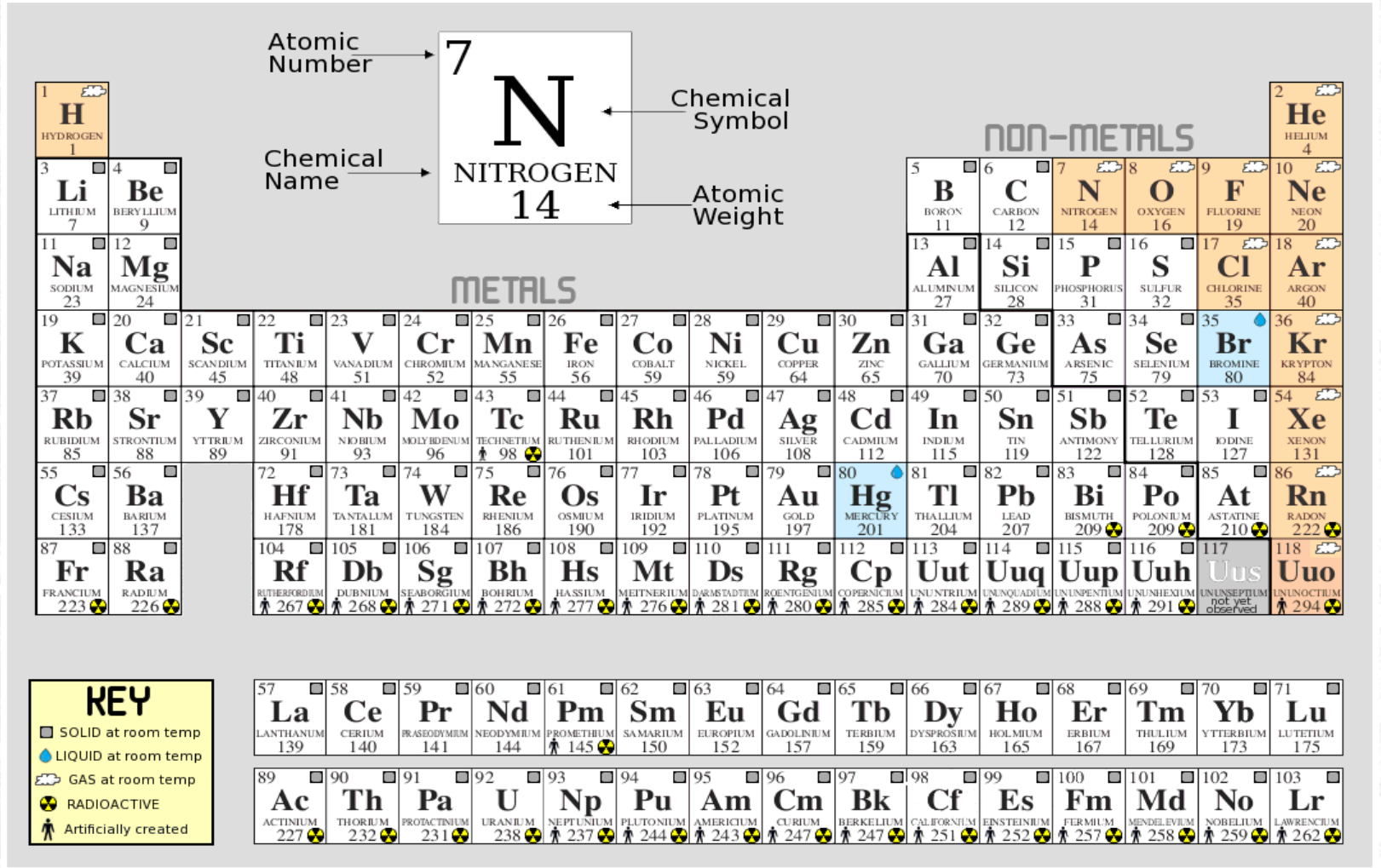
What are the actuators behind the trends and patterns that are invisible to the human eye?





A role model: The Periodic Table of Elements

Amazing … but much simpler



Dmitri Mendeleev
(1834-1907)

http://www.wpclipart.com

What is Artificial Intelligence?

Terminology …

Artificial Intelligence

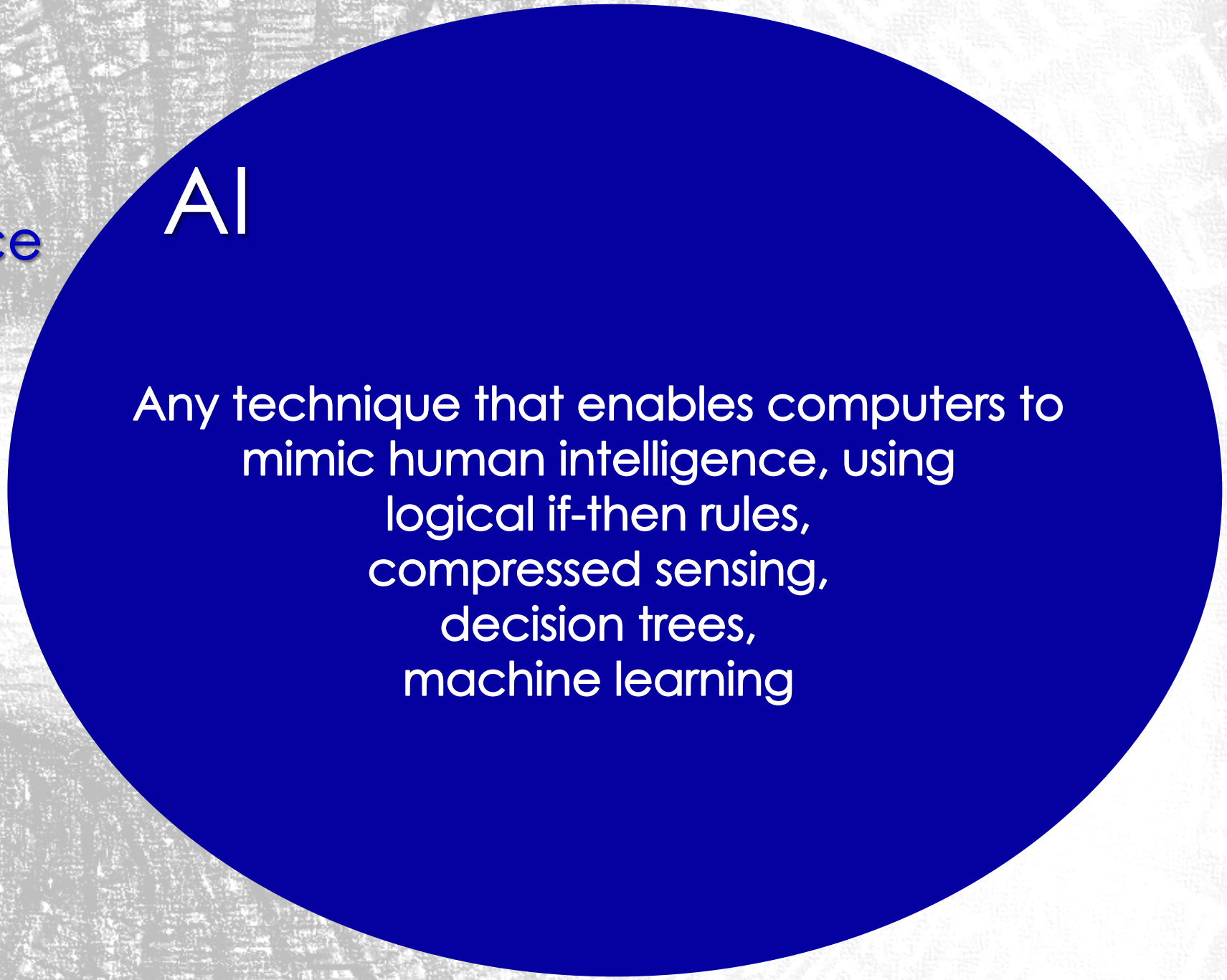
- Born 1956
- Slowed down …
- Now big revival

Machine learning

- What everyone has always been doing

Deep learning

- What everyone wants to do



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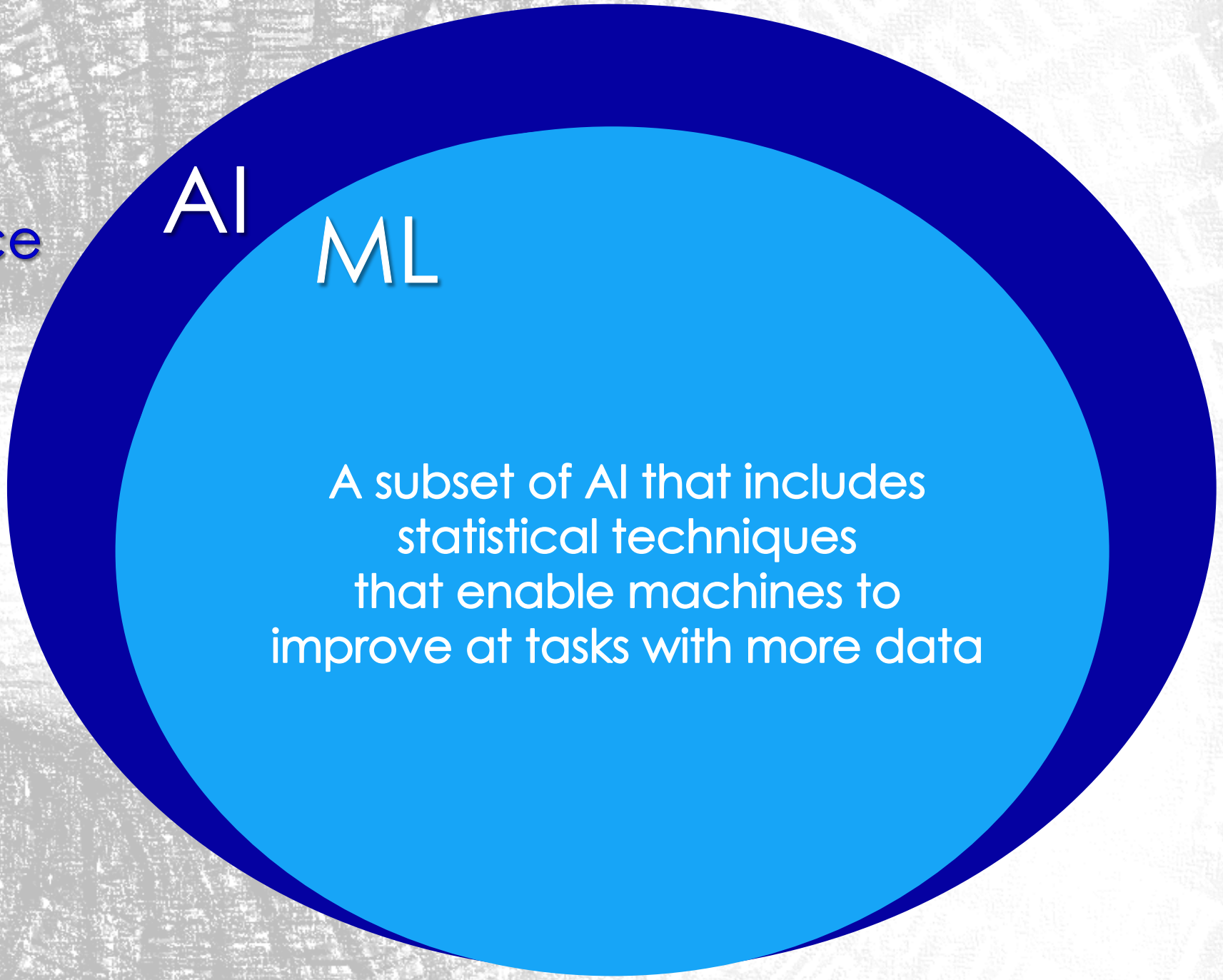

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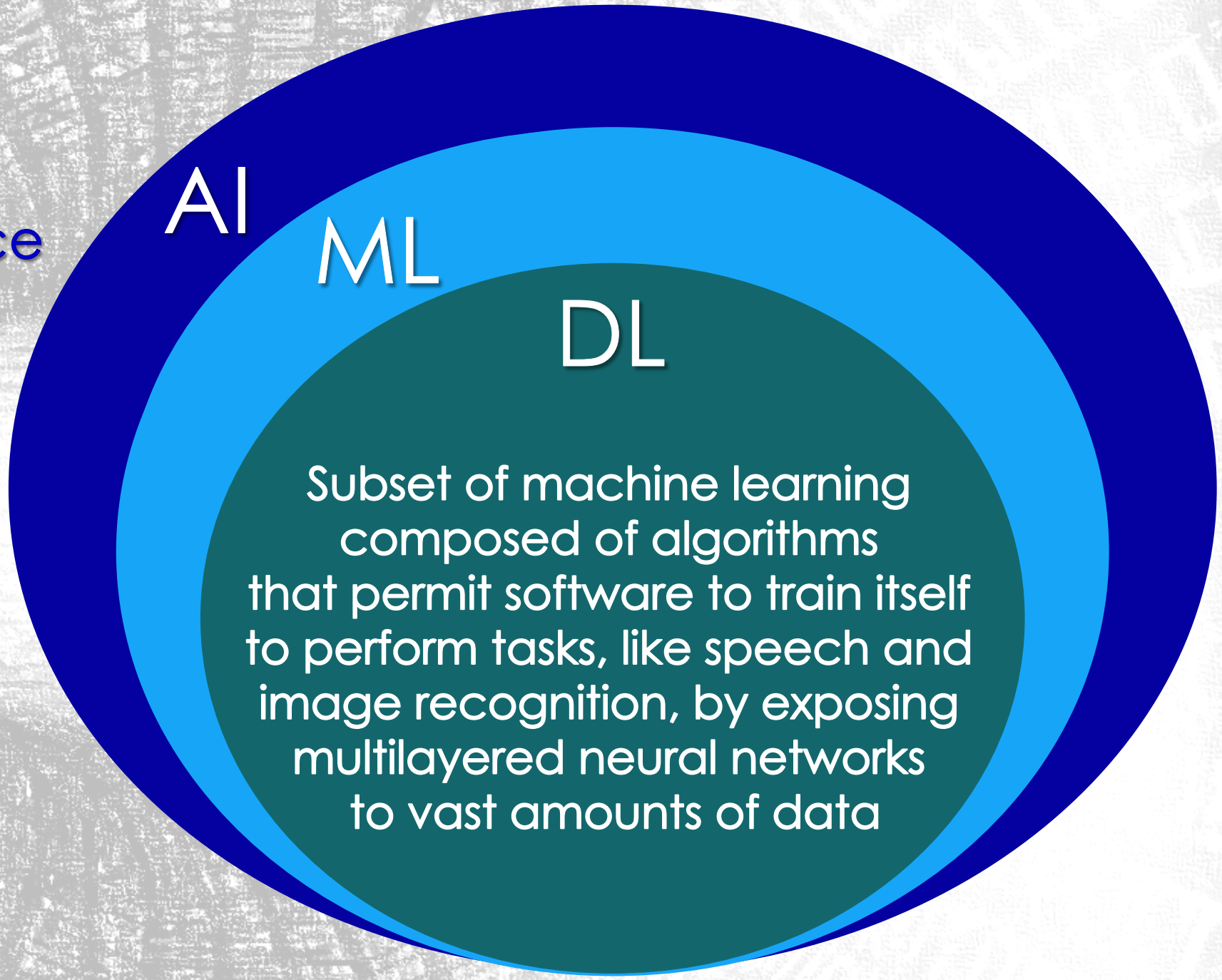


Developments in many areas – **many tools**

Computer Science

Cheminformatics

Knowledge Graphs

Clustering

Compressed Sensing

Linguistics

Neural Networks

Signal Processing

Subgroup Discovery

Social media

Kernel Ridge Regression

Robotics

Bioinformatics

Support Vector Machines

Random Forest

Intelligent Systems

and more …

More maps ...

Crystal-structure prediction

- Octet binaries
- $Al_xGa_yIn_zO_3$
- Perovskites

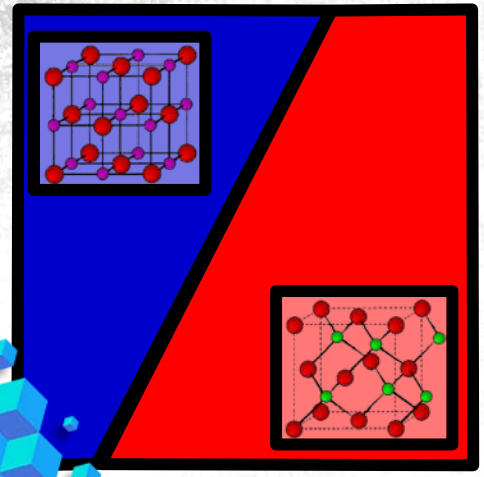
Property classification

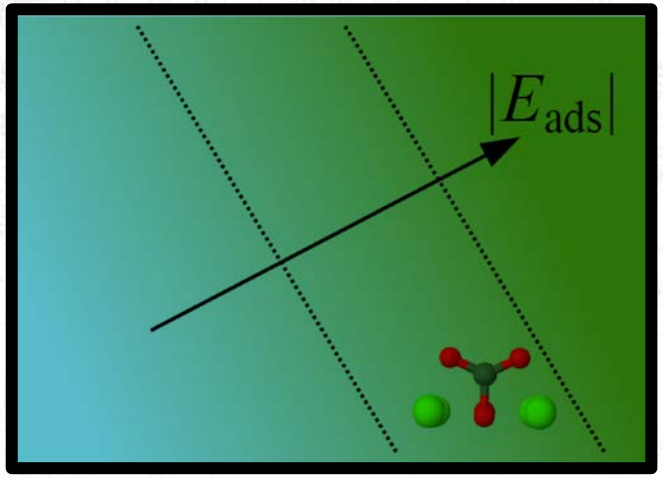
- Metal vs. insulator
- Topological insulators

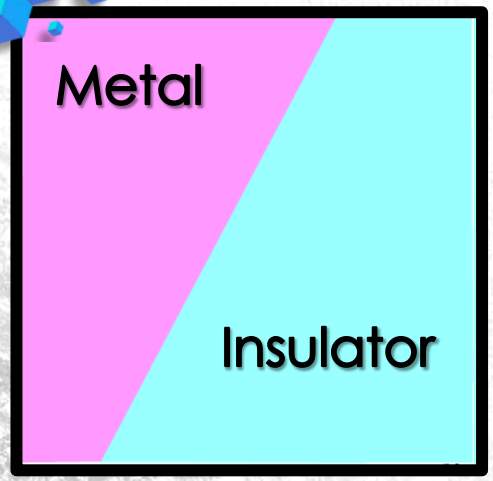
https://analytics-toolkit.nomad-coe.eu/

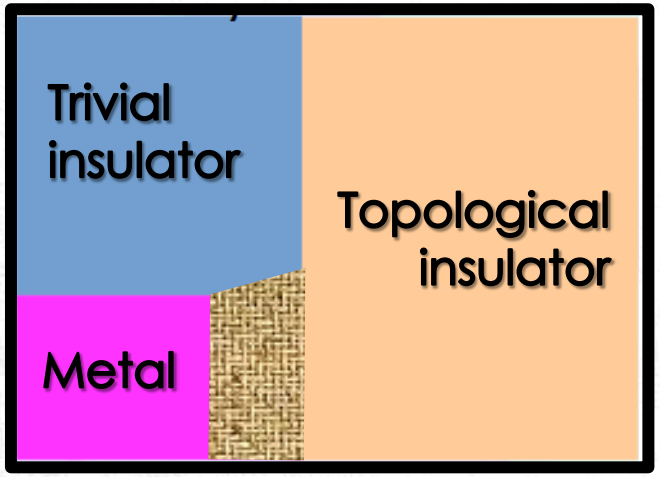
NOMAD

Activation of CO_2 at metal oxides and carbides









M. Scheffler's group, FHI Berlin

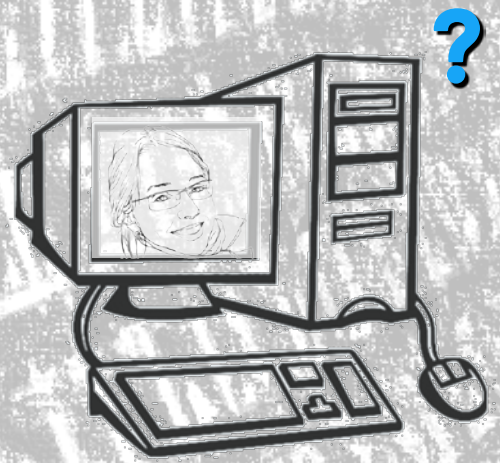
What do we need for the Big Picture?

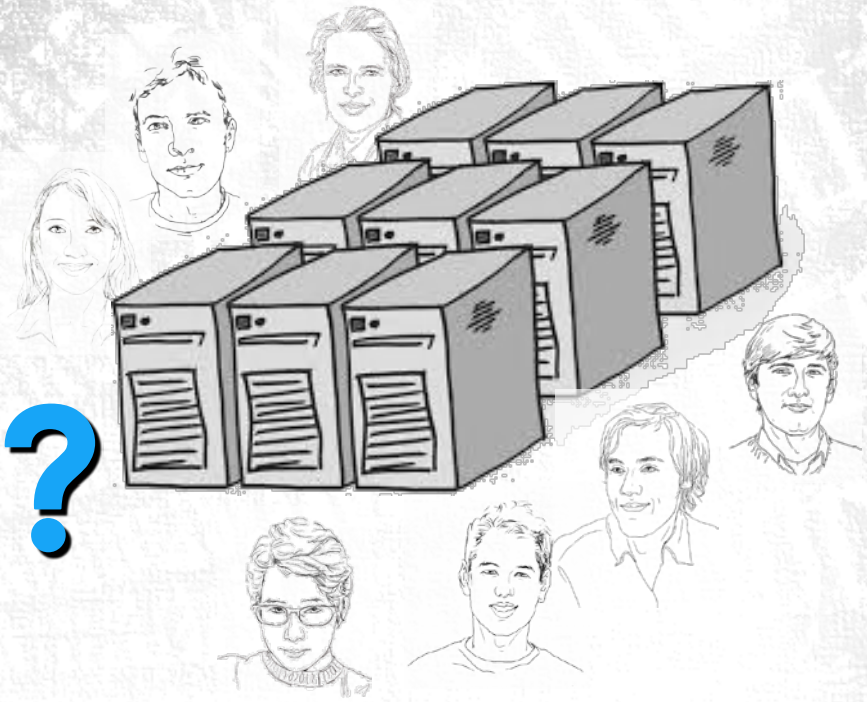
FAIR data infrastructures

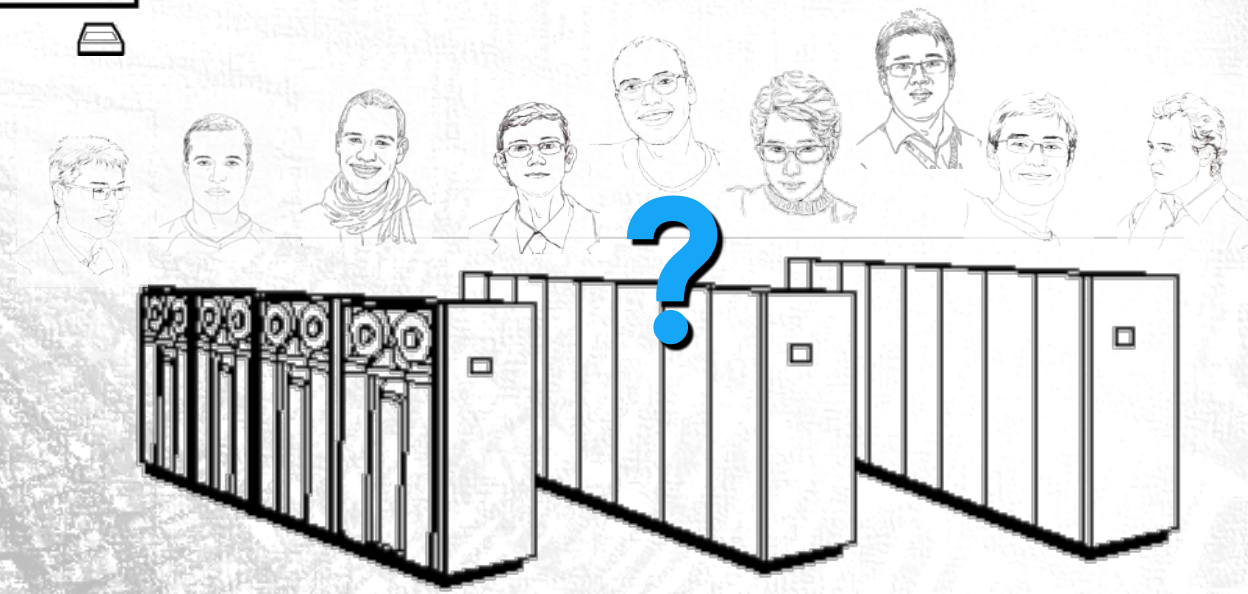
M. Wilkinson et al., Sci. Data(2016).

Findable

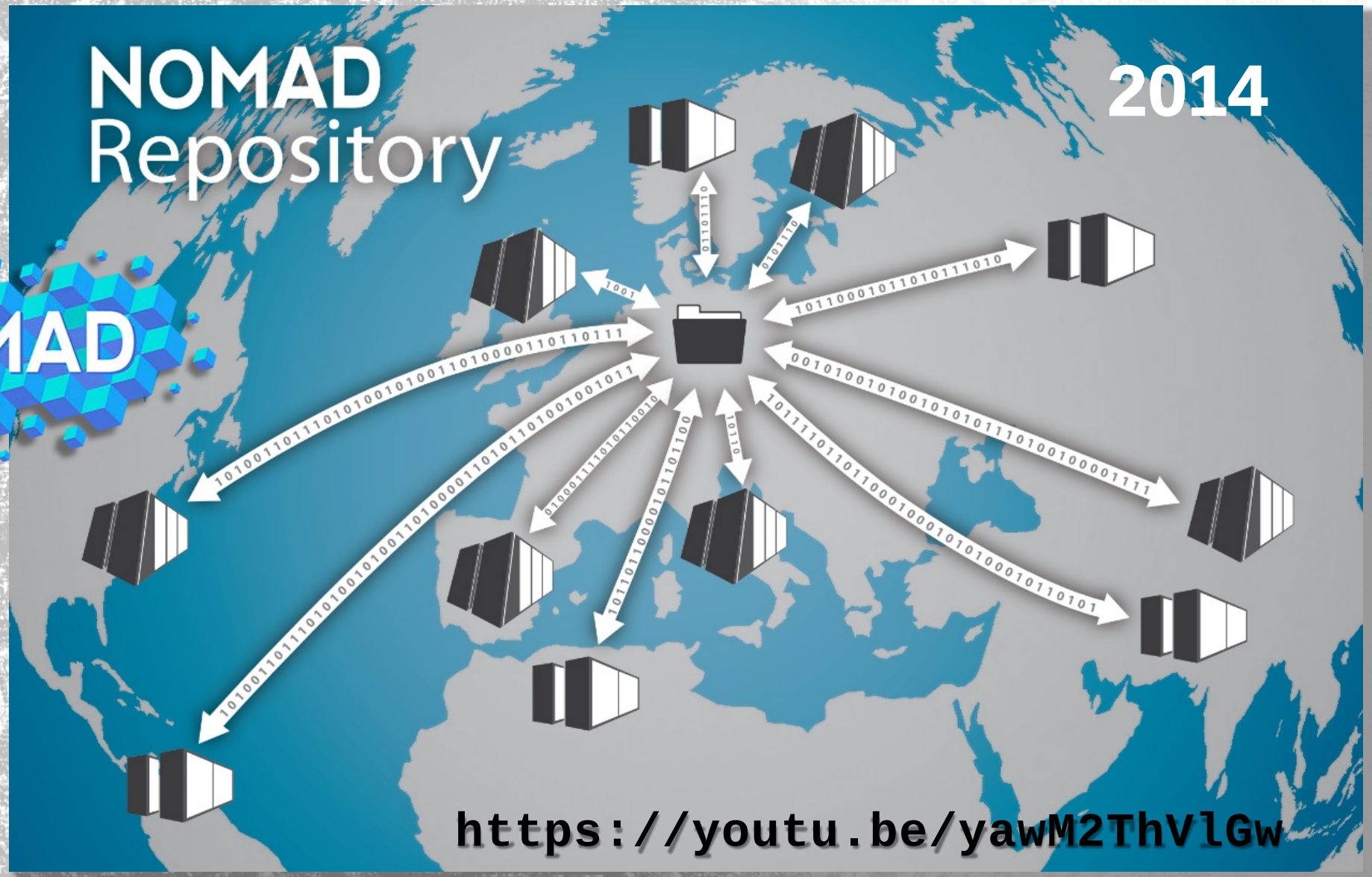
Findable?





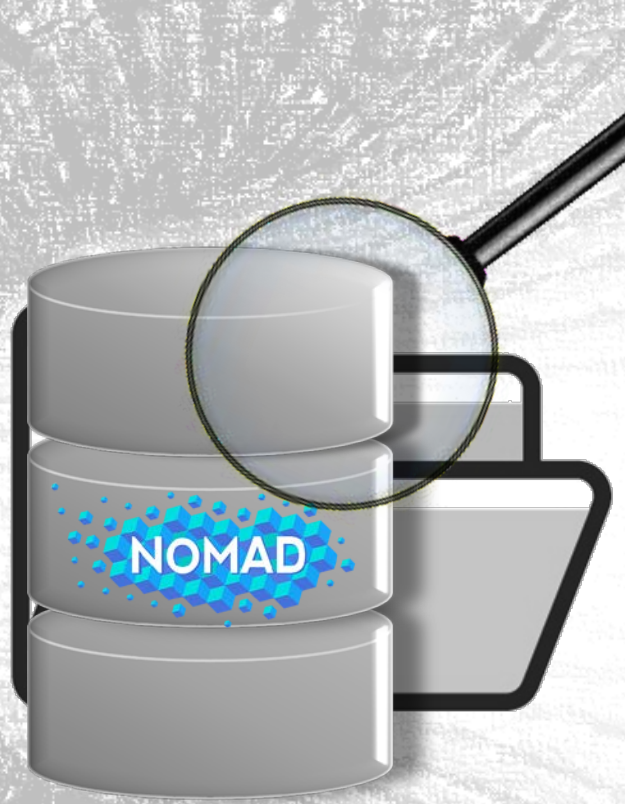


Novel Materials Discovery …



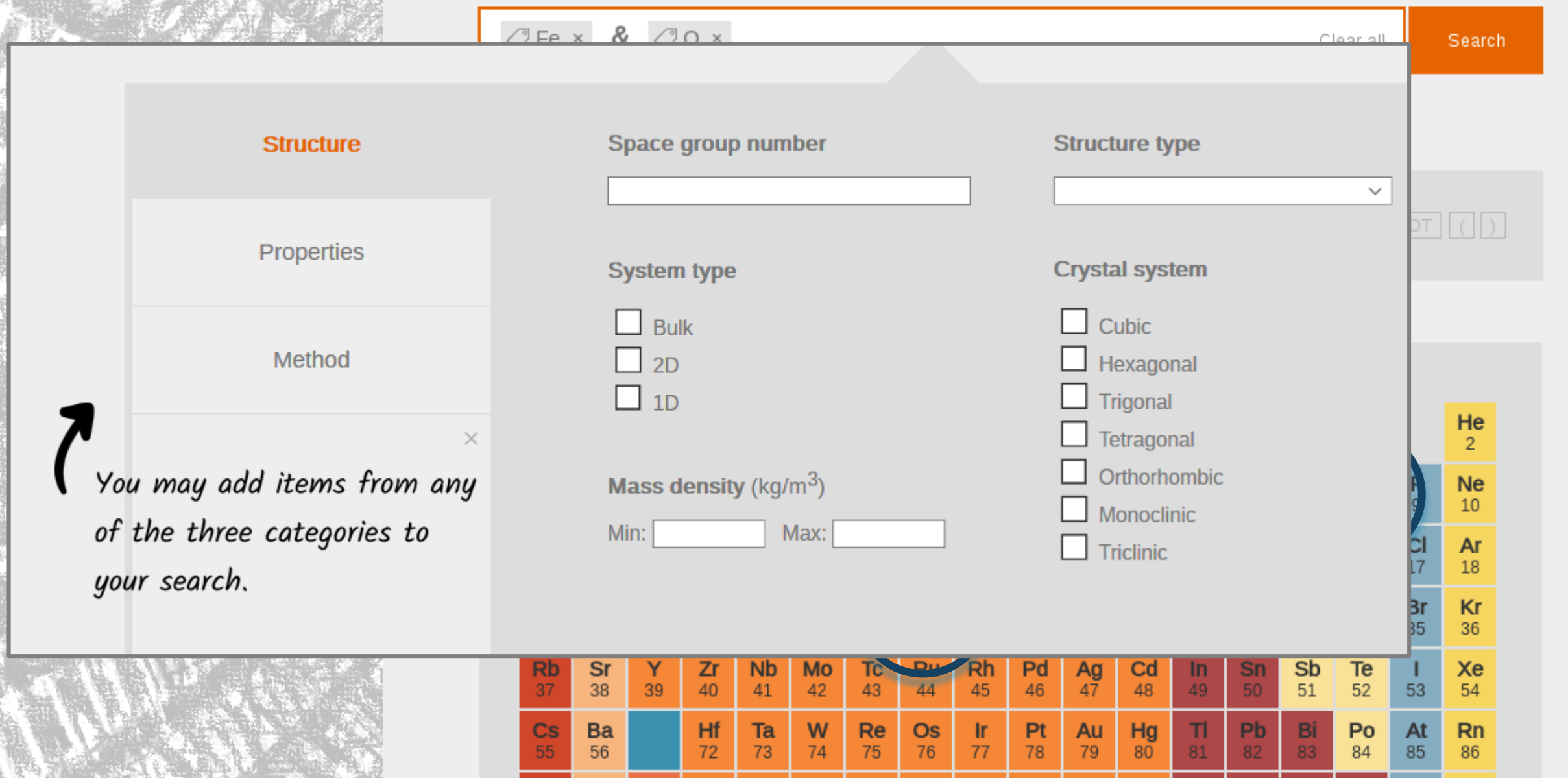
Accessible

Accessible?



The NOMAD Encyclopedia

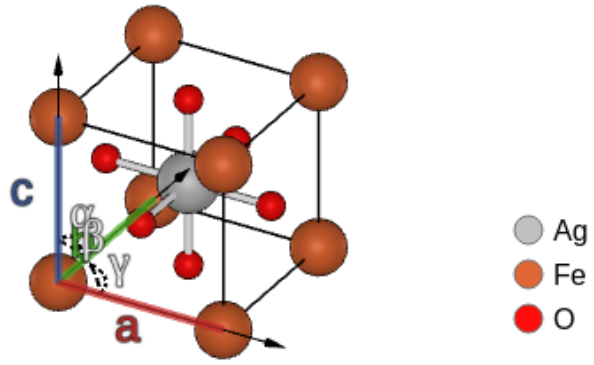
https://encyclopedia.nomad-coe.eu/



Overview page

$AgFeO_3$ - space group 221

Structure



Show axis Show bonds Virtual Reality files

System type: bulk

Space group: 221

Structure type: CaO3Ti (Cubic Perovskite)

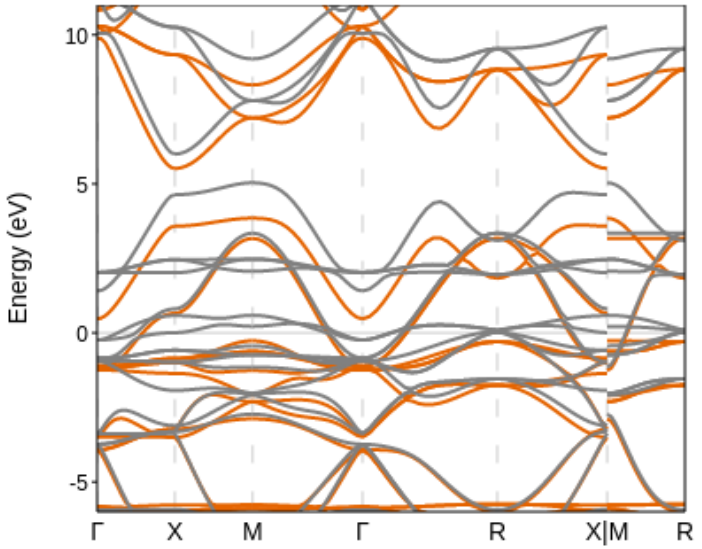
Methodology

Available calculations

Functional	Code
7 GGA	7 VASP

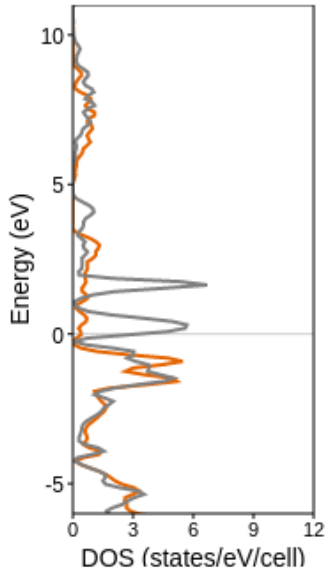
Electronic structure

Band structure



From calculation **1648548**
(GGA - VASP)

DOS



From calculation **383297**
(GGA - VASP)

Spin ⇧ Spin ⇩

https://encyclopedia.nomad-coe.eu/

Thermal properties

Introduction to NOMAD Encyclopedia | The NOMAD Laboratory | Guest (LOGIN)

NOMAD Encyclopedia

Additional information

Search > Overview > Thermal Properties

Ge - space group 227

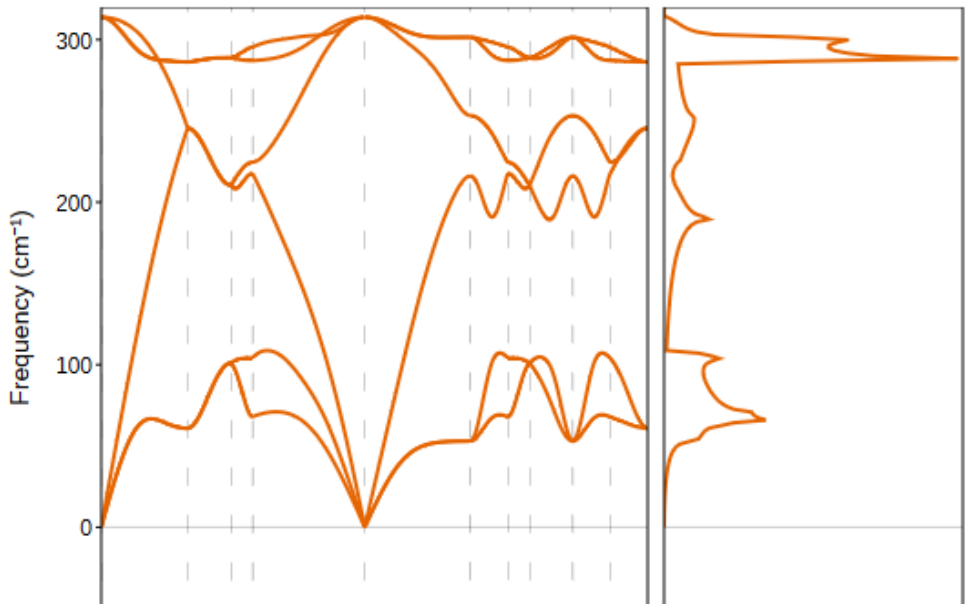
Calculations

- Germanium
  - GGA
  - LDA
    - FHI-aims (484)
      - 232721
      - 240305
      - 245463
      - 248199
      - 247902
      - 334303

Vibrational and thermal properties

922350

Phonon dispersion



Phonon DOS

Understanding and learning similarity

M. Kuban

Can we find materials similar in terms of

- Structure ?
- Properties ?
- Function ?

How do they correlate?

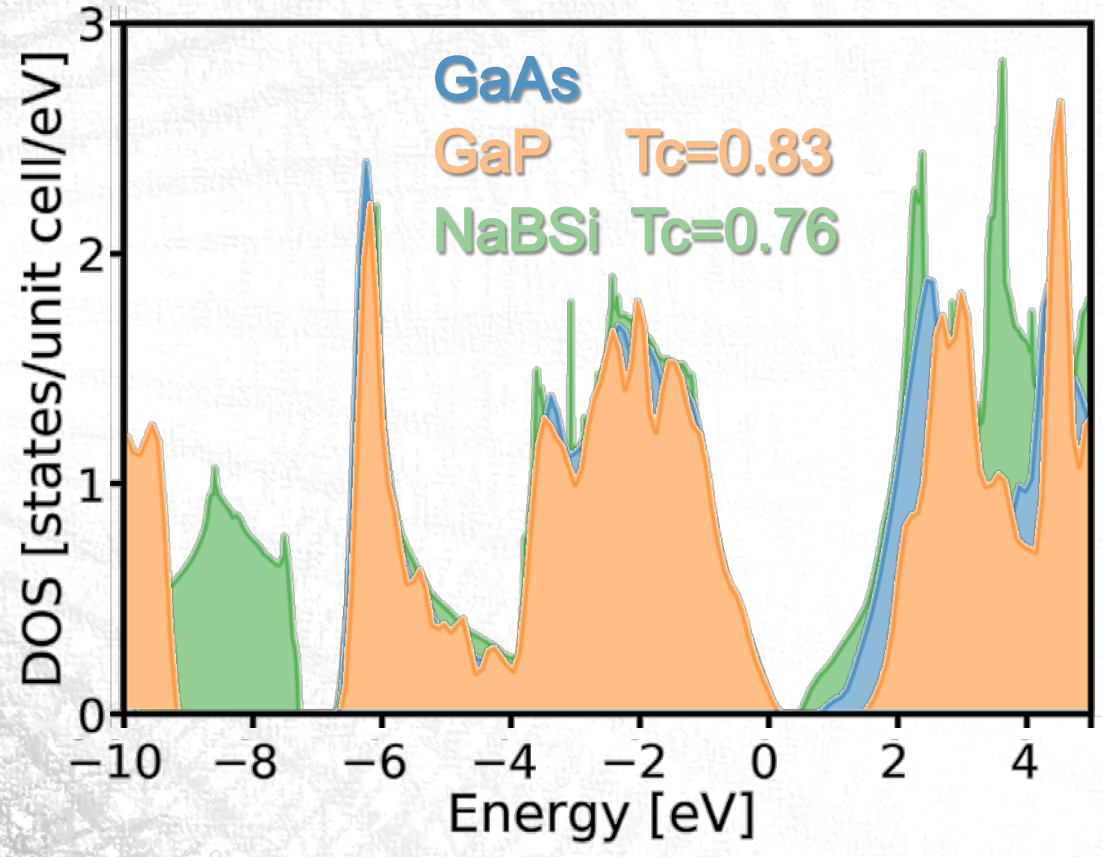
Electronic-structure fingerprints

M. Kuban

Similarity in terms of features in density-of-states

Tc ∈ [0,1] … similarity coefficient

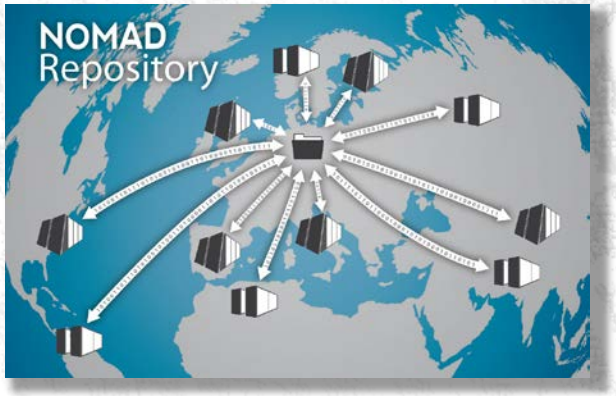
O. Isayev et al., Chem. Mater. 27, 735 (2015).



Based on 280 000 materials downloaded through the Ecnyclopedia API

Interoperable

The NOMAD Archive



More than 56 million calculations coming from …

- 40 different codes

Normalized data

- Unified format, units, …

Metadata

- Crucially important
- Unique description of data
  - Every output fully parsed

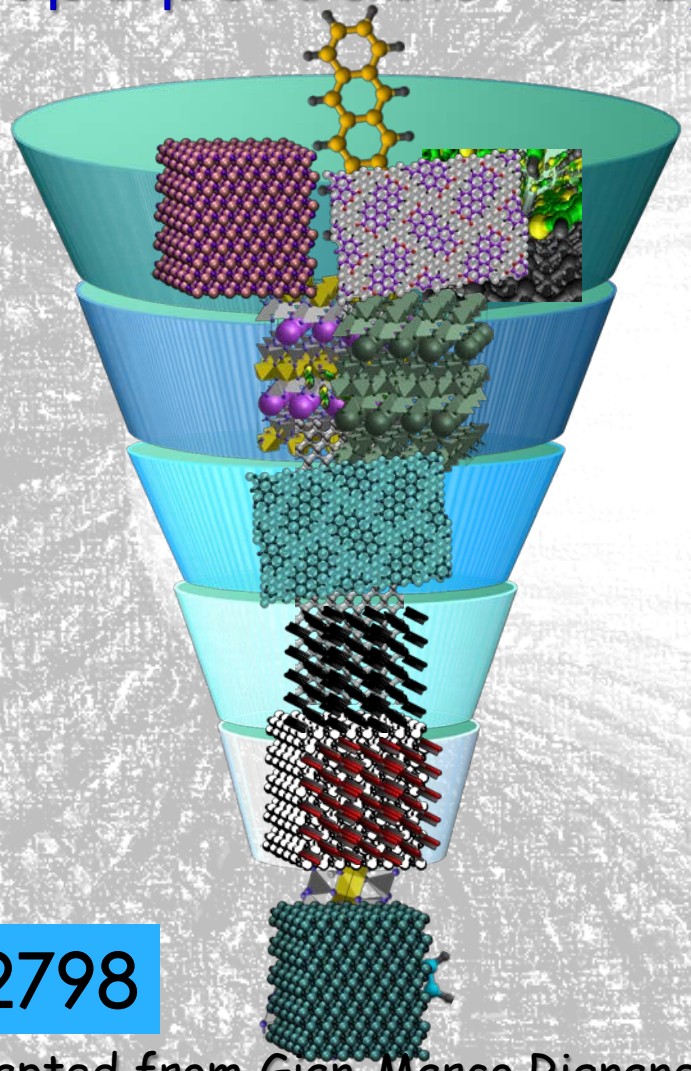
Ry, kcal/mol eV, J, …?

Quality control
Error quantification

Reusable

High-throughput screening

Reusable = repurposeable = *recyclable*



Property 1

Property 2

Property 3

Property 4

Property 5

12798

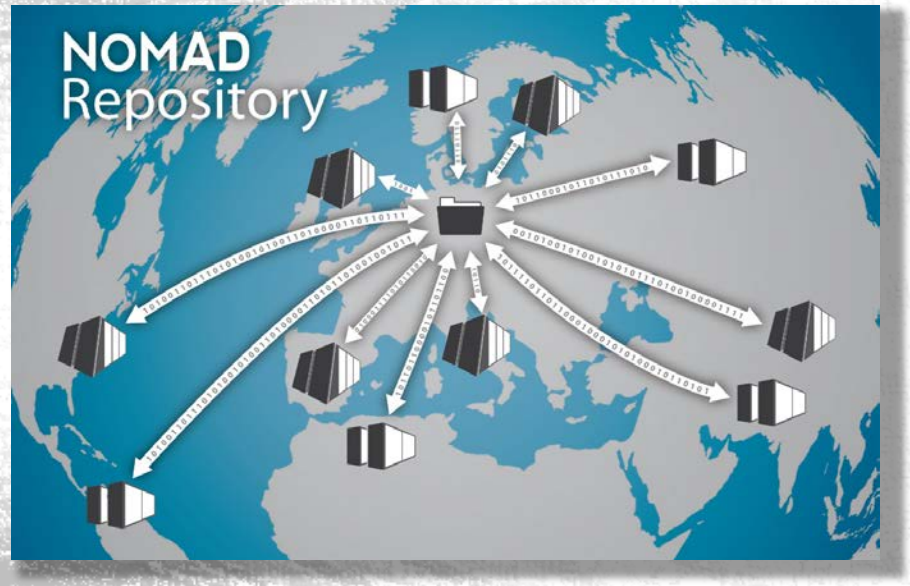
3

Animation adopted / adapted from Gian-Marco Rignanese

Next steps … …

From the beginning …

Matthias Scheffler
FHI Berlin



Claudia Draxl
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Pintail Dublin

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DTU Lyngby

Kimmo Koski
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Kings College London

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Stefan Heinzel
MPSCD Garching

Dieter Kranzlmüller
LRZ Munich

Francesc Illas
Univ. Barcelona

Jose Maria Cela
BSC Barcelona

Funding from the European Union's Horizon 2020 research and innovation programme, grant agreement No 676580.

Next steps

NOMAD is an Implementation Network at GO FAIR

https://www.go-fair.org/, an international approach for the practical implementation of the European Open Science Cloud (EOSC).

FAIR-DI

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

https://fairdi.eu

WELCOME

Computational materials science - NOMAD

Experimental materials science

Soft-matter and biomolecular simulations

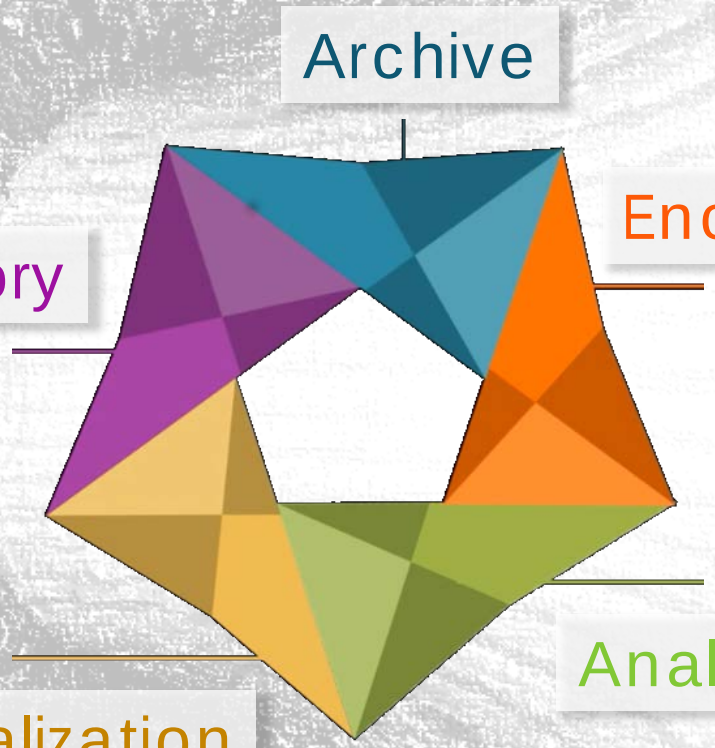
Heterogeneous catalysis

Astronomy and space-situational awareness

Artificial-intelligence tools

Digital research infrastructures

Thanks !!



FAIR-DI

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