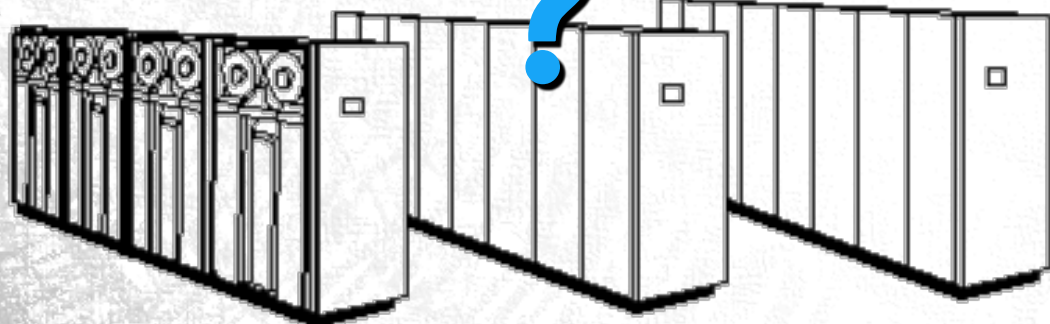
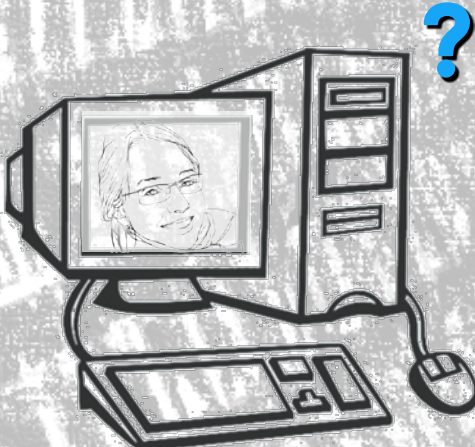




**NOMAD**

**Claudia Draxl**

# Should we care?

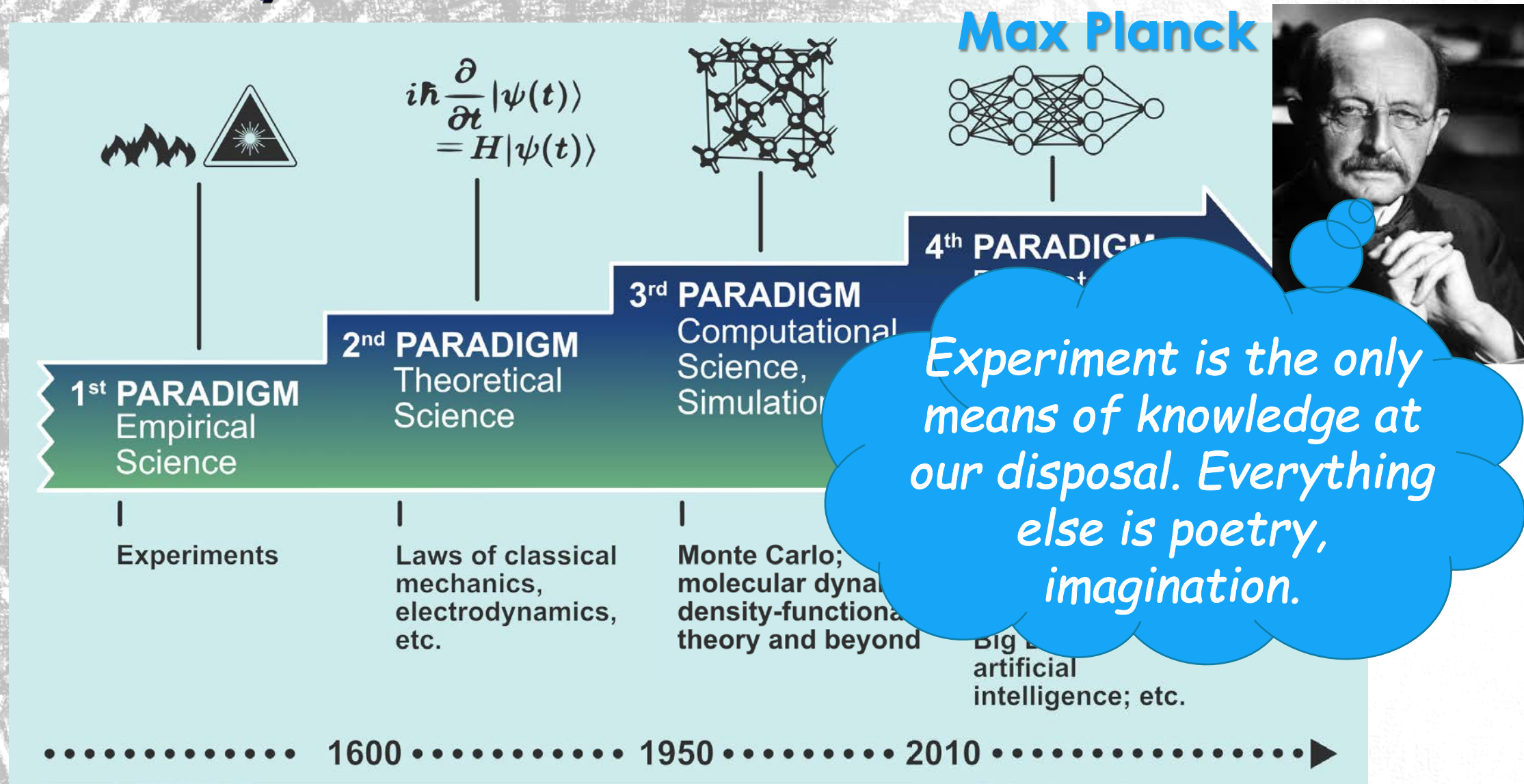


The image features a collage of scientific and technological scenes. At the top, a large, faint, textured pattern of interconnected lines and dots, resembling a molecular or network structure, spans the width. Below this, a dark blue banner contains the logo 'MRS' in white, with each letter in a separate square, followed by the text 'MATERIALS RESEARCH SOCIETY®' in white. The main body of the image is a collage of three scenes: on the left, a scientist in a white lab coat and safety glasses works with a microscope; in the center, a woman in a lab coat looks up at a large array of solar panels; on the right, a man in a lab coat and safety glasses works with a piece of scientific equipment, with a woman in the background looking at a tablet. The bottom of the image is a dark blue banner with white text.

**MRS** MATERIALS RESEARCH SOCIETY®

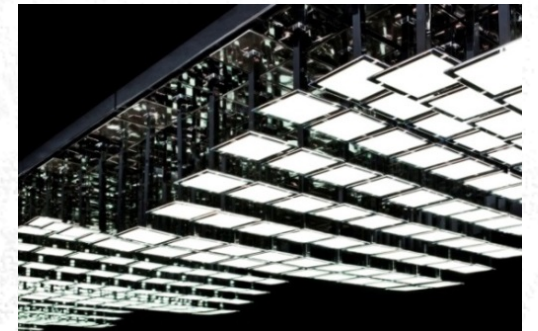
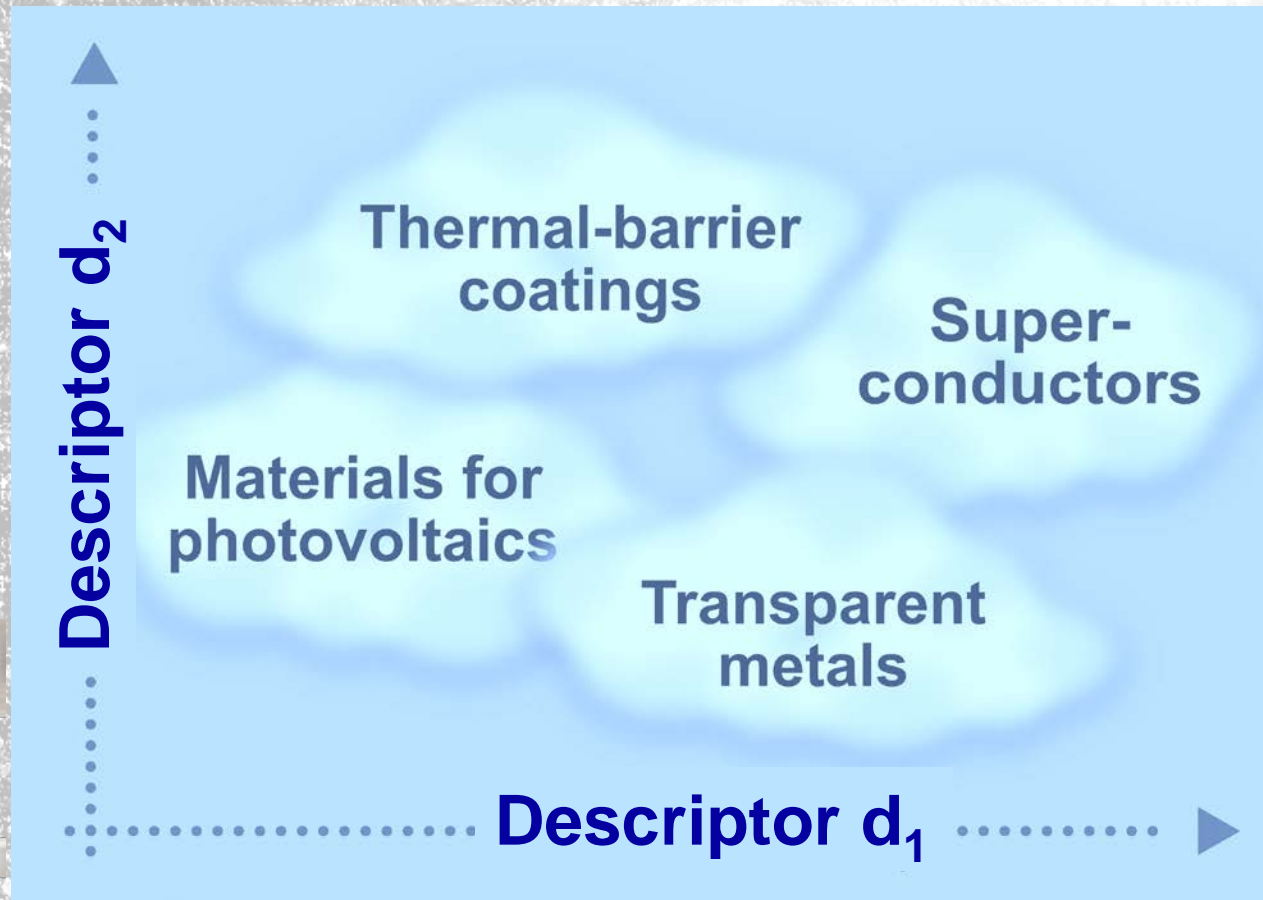
Advancing materials.  
Improving the quality of life.

# From history to future ...



# Our scientific vision ...

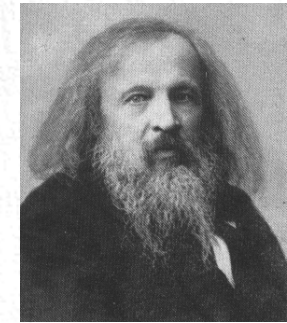
What are the actuators behind the trends and patterns that are invisible to the human eye?



# A role model: The Periodic Table of Elements

Amazing ... but much simpler

Atomic Number → 7																		Chemical Symbol → N						
Chemical Name → NITROGEN																		Atomic Weight → 14						
METALS																		NON-METALS						
1 H HYDROGEN 1	3 Li LITHIUM 7		4 Be BERYLLIUM 9																	2 He HELIUM 4				
11 Na SODIUM 23	12 Mg MAGNESIUM 24																	5 B BORON 11	6 C CARBON 12	7 N NITROGEN 14	8 O OXYGEN 16	9 F FLUORINE 19	10 Ne NEON 20	
19 K POTASSIUM 39	20 Ca CALCIUM 40	21 Sc SCANDIUM 45	22 Ti TITANIUM 48	23 V VANADIUM 51	24 Cr CHROMIUM 52	25 Mn MANGANESE 55	26 Fe IRON 56	27 Co COBALT 59	28 Ni NICKEL 59	29 Cu COPPER 64	30 Zn ZINC 65	31 Ga GALLIUM 70	32 Ge GERMANIUM 73	33 As ARSENIC 75	34 Se SELENIUM 79	35 Br BROMINE 80	36 Kr KRYPTON 84							
37 Rb RUBIDIUM 85	38 Sr STRONTIUM 88	39 Y YTTRIUM 89	40 Zr ZIRCONIUM 91	41 Nb NIOBIUM 93	42 Mo MOLYBDENUM 96	43 Tc TECHNETIUM 98	44 Ru RUTHENIUM 101	45 Rh RHODIUM 103	46 Pd PALLADIUM 106	47 Ag SILVER 108	48 Cd CADMIUM 112	49 In INDIUM 115	50 Sn TIN 119	51 Sb ANTIMONY 122	52 Te TELLURIUM 128	53 I IODINE 127	54 Xe XENON 131							
55 Cs CESIUM 133	56 Ba BARIUM 137																	80 Hg MERCURY 201	81 Tl THALLIUM 204	82 Pb LEAD 207	83 Bi BISMUTH 209	84 Po POLONIUM 209	85 At ASTATINE 210	86 Rn RADON 222
87 Fr FRANCIUM 223	88 Ra RADIUM 226																	89 Uut UNUNTRIUM 284	90 Uuq UNUNQUADIUM 289	91 Uup UNUNPENTIUM 288	92 Uuh UNUNHEXIUM 291	93 Uus UNUNSEPTIUM not yet discovered	94 Uuo UNUNOCTIUM 294	
<b>KEY</b> ■ SOLID at room temp ● LIQUID at room temp ☁ GAS at room temp ☢ RADIOACTIVE ⚗ Artificially created																								
57 La LANTHANUM 139	58 Ce CERIUM 140	59 Pr PRASEODYMIUM 141	60 Nd NEODYMIUM 144	61 Pm PROMETHIUM 145	62 Sm SAMARIUM 150	63 Eu EUROPIUM 152	64 Gd GADOLINIUM 157	65 Tb TERBIUM 159	66 Dy DYSPROSIUM 163	67 Ho HOLMIUM 165	68 Er ERBIUM 167	69 Tm THULIUM 169	70 Yb YTTERIUM 173	71 Lu LUTETIUM 175										
89 Ac ACTINIUM 227	90 Th THORIUM 232	91 Pa PROTACTINIUM 231	92 U URANIUM 238	93 Np NEPTUNIUM 237	94 Pu PLUTONIUM 244	95 Am AMERICIUM 243	96 Cm CURIUM 247	97 Bk BERKELIUM 247	98 Cf CALIFORNIUM 251	99 Es EINSTEINIUM 252	100 Fm FERMIUM 257	101 Md MENDELEVIUM 258	102 No NOBELIUM 259	103 Lr LAWRENCIUM 262										



Dmitri Mendeleev  
(1834-1907)

# What is Artificial Intelligence?

The background of the slide is a complex, abstract pattern. It features a grid-like structure that appears to be a stylized representation of a brain or a neural network. The grid is composed of many small, interconnected nodes and lines, creating a dense, textured appearance. The colors are primarily shades of gray and white, with some darker areas that suggest depth and shadow. The overall effect is one of a highly structured, yet organic-looking system.

# 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

# AI

Any technique that enables computers to mimic human intelligence, using logical if-then rules, compressed sensing, decision trees, machine learning



# 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

AI

ML

A subset of AI that includes  
statistical techniques  
that enable machines to  
improve at tasks with more data

# Terminology ...

## Artificial Intelligence

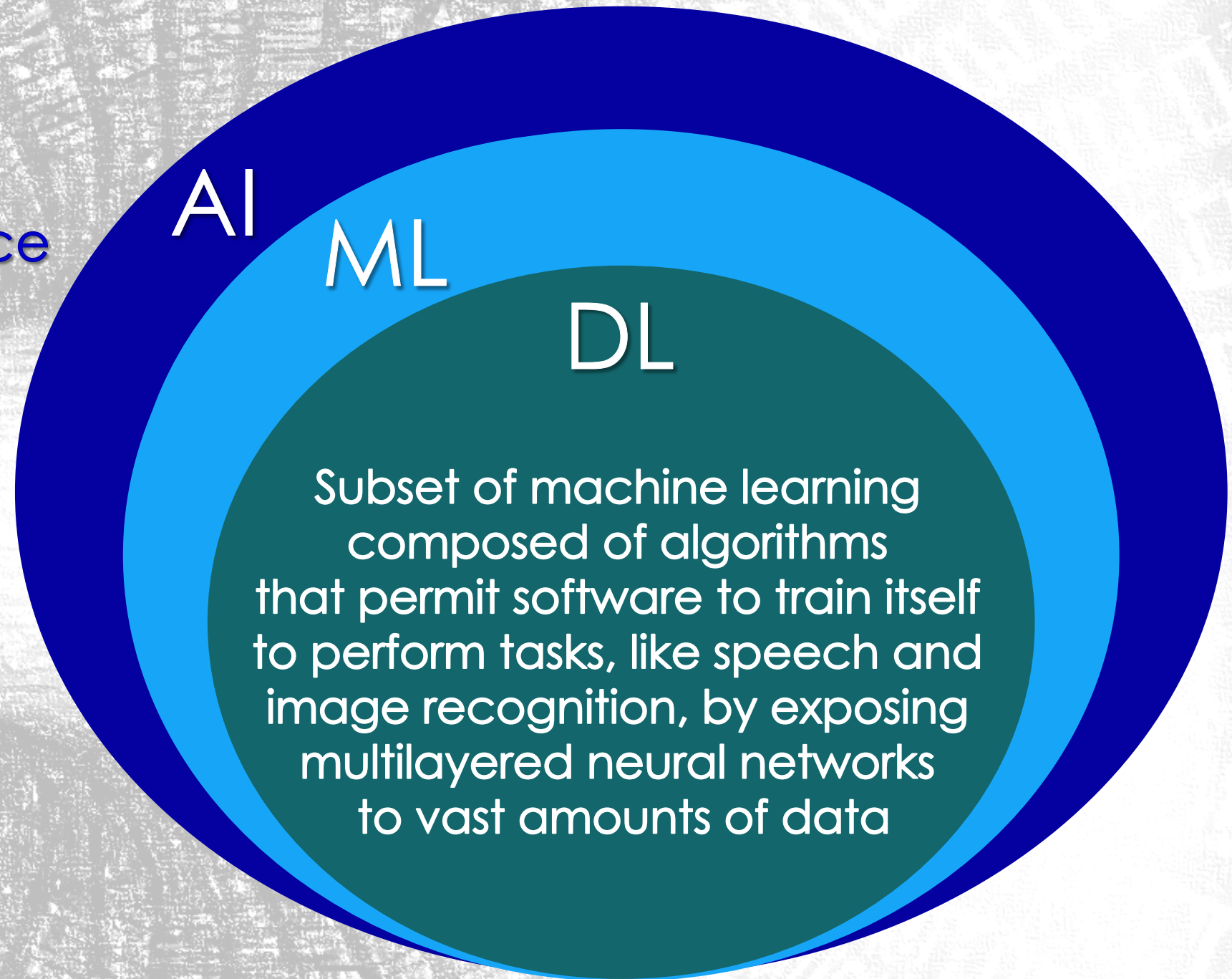
Born 1956  
Slowed down ...  
Now big revival

## Machine learning

What everyone  
has always  
been doing

## Deep learning

What everyone  
wants to do



# Developments in many areas – many tools

Cheminformatics

Computer Science

Clustering

Knowledge Graphs

Neural Networks

Compressed Sensing

Linguistics

Signal Processing

Subgroup Discovery

Kernel Ridge Regression

Social media

Bioinformatics

Robotics

Support Vector Machines

Random Forest

Intelligent Systems

and more ...

# More maps ...

## Crystal-structure prediction

Octet binaries

$\text{Al}_x\text{Ga}_y\text{In}_z\text{O}_3$

Perovskites



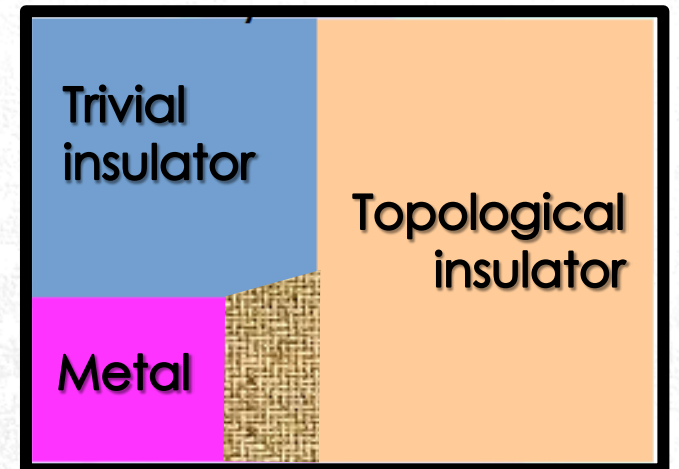
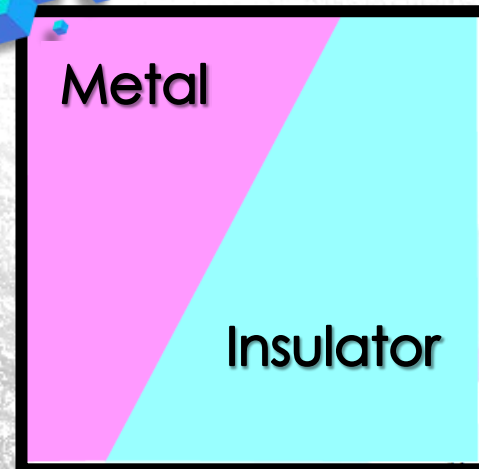
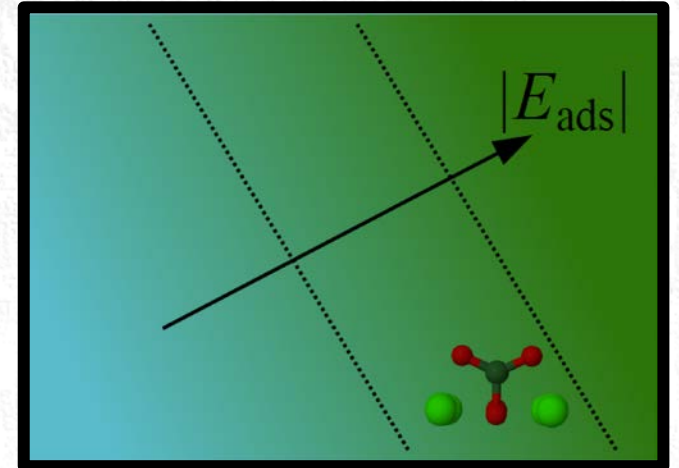
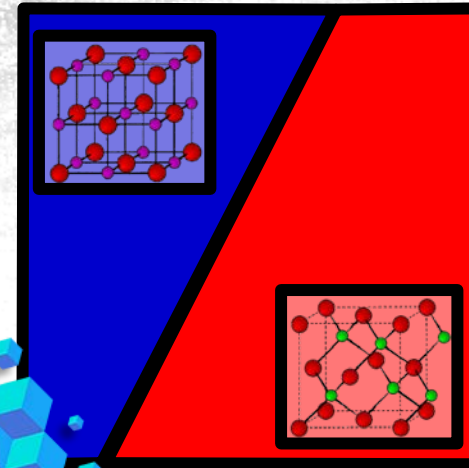
## Property classification

Metal vs. insulator

Topological insulators

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

## Activation of $\text{CO}_2$ at metal oxides and carbides



What do we need for the **Big Picture**?



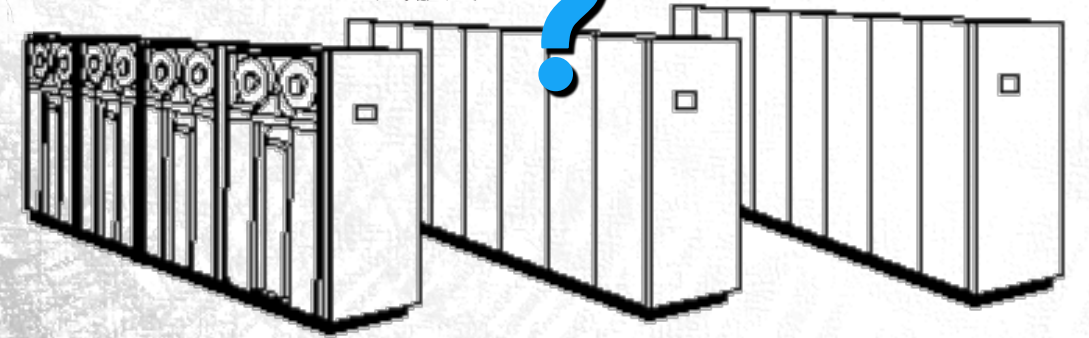
**FAIR**

**data infrastructures**



**F**indable

# Findable?



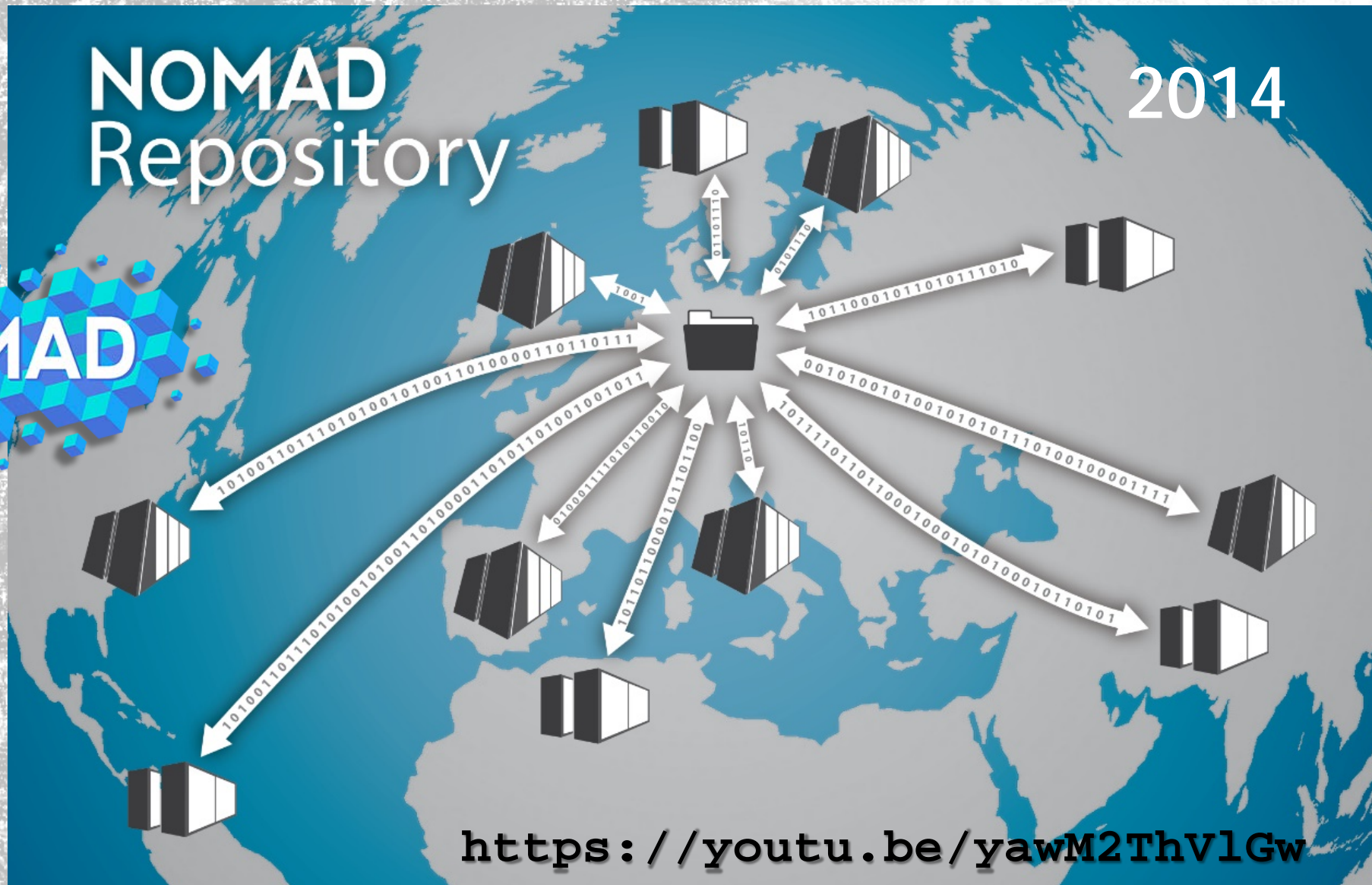
# Novel Materials Discovery ...

NOMAD  
Repository

2014

NOMAD

<https://youtu.be/yawM2ThVlGw>

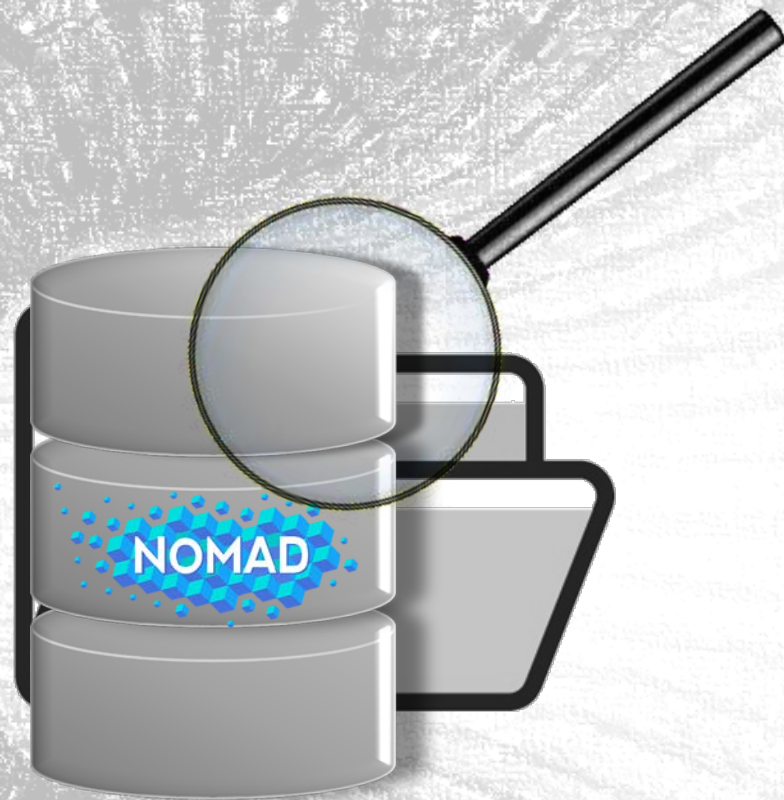




A grayscale photograph of a tunnel with a bright light at the far end, creating a strong perspective. The tunnel walls are textured and the floor is dark. The light at the end is very bright, creating a lens flare effect.

**A**ccessible

# Accessible?



# The NOMAD Encyclopedia

The screenshot shows the NOMAD Encyclopedia search interface. At the top, there is a search bar with the text "Fe x & O x" and a "Clear all" button. To the right is an orange "Search" button. Below the search bar is a grey overlay containing search filters. On the left side of the overlay, there are three categories: "Structure", "Properties", and "Method". An arrow points from the text "You may add items from any of the three categories to your search." to these categories. The "Structure" category is expanded, showing several filter options:

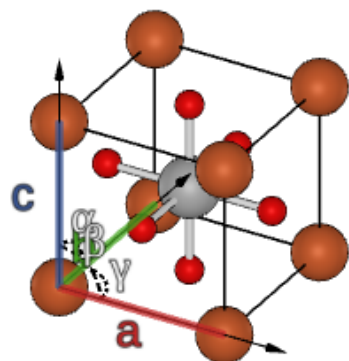
- Space group number:
- Structure type:
- System type:
  - Bulk
  - 2D
  - 1D
- Mass density (kg/m<sup>3</sup>):  
Min:  Max:
- Crystal system:
  - Cubic
  - Hexagonal
  - Trigonal
  - Tetragonal
  - Orthorhombic
  - Monoclinic
  - Triclinic

At the bottom of the screenshot, a portion of the periodic table is visible, showing elements from Rb (37) to Xe (54) in the top row and Cs (55) to Rn (86) in the bottom row.

# Overview page

## AgFeO<sub>3</sub> - 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

7 GGA

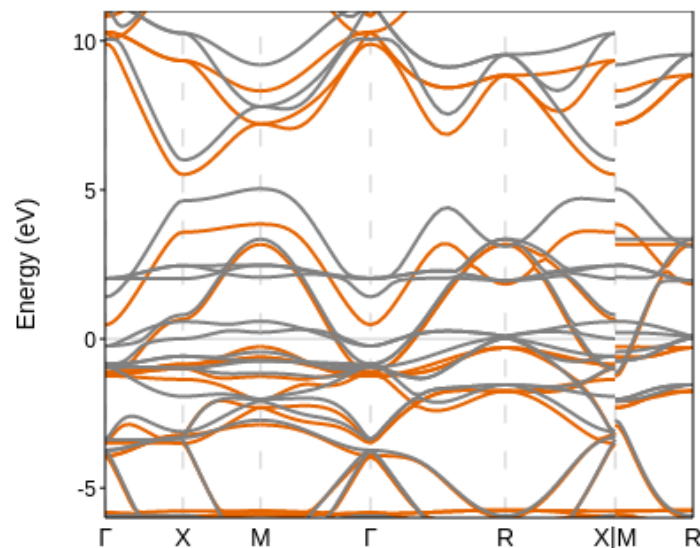
Code

7 VASP

### Electronic structure



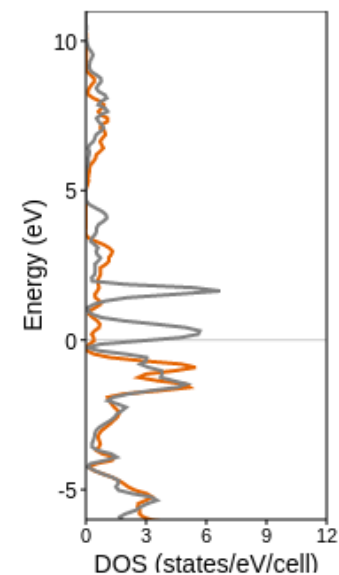
#### Band structure



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

— Spin ↑ — Spin ↓

#### DOS



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

# Thermal properties

Introduction to NOMAD Encyclopedia

The NOMAD Laboratory



Guest ([LOGIN](#))



NOMAD Encyclopedia

Additional information

Search > Overview > Thermal Properties

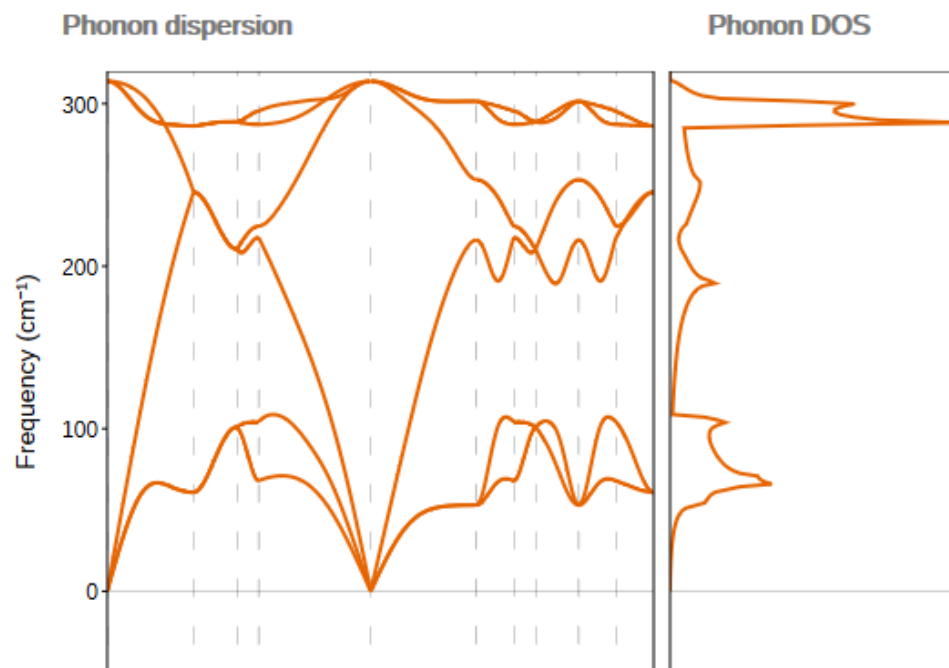
## Ge - space group 227

### Calculations

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

### Vibrational and thermal properties

922350



# Understanding and learning similarity

Can we find materials similar in terms of

Structure ?

Properties ?

Function ?

How do they correlate?



**M. Kuban**

# Electronic-structure fingerprints

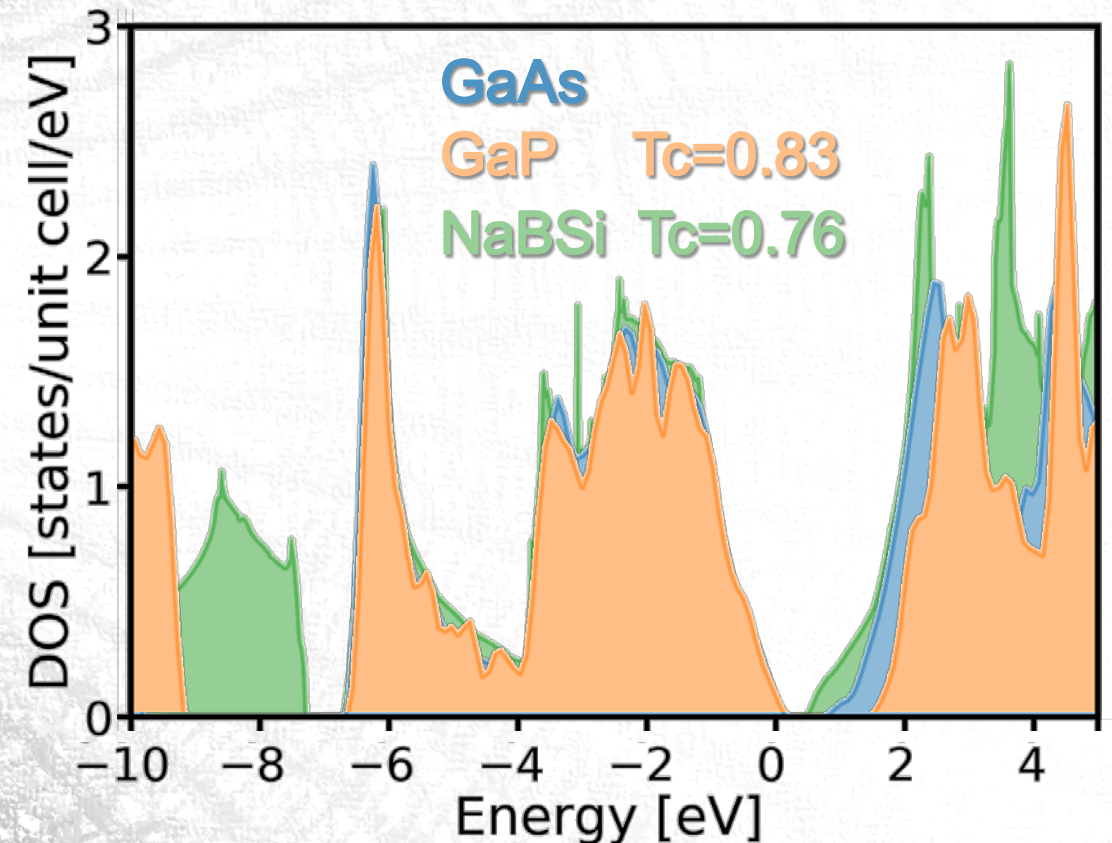


M. Kuban

Similarity in terms of features in density-of-states

$T_c \in [0,1]$  ... similarity coefficient

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



Based on 280 000 materials downloaded through the Ecnyclopedia API



**I**nteroperable



# The NOMAD Archive

More than 56 million calculations coming from ...

40 different codes

Normalized data

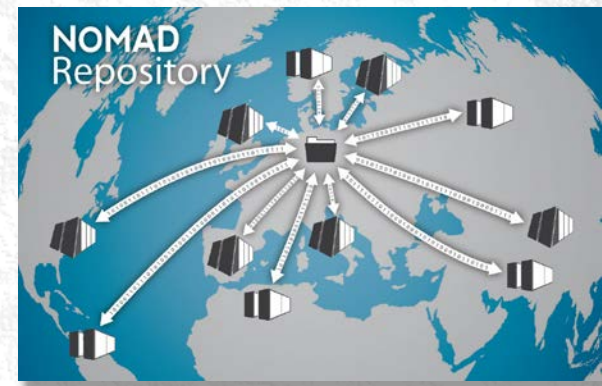
Unified format, units, ...

Metadata

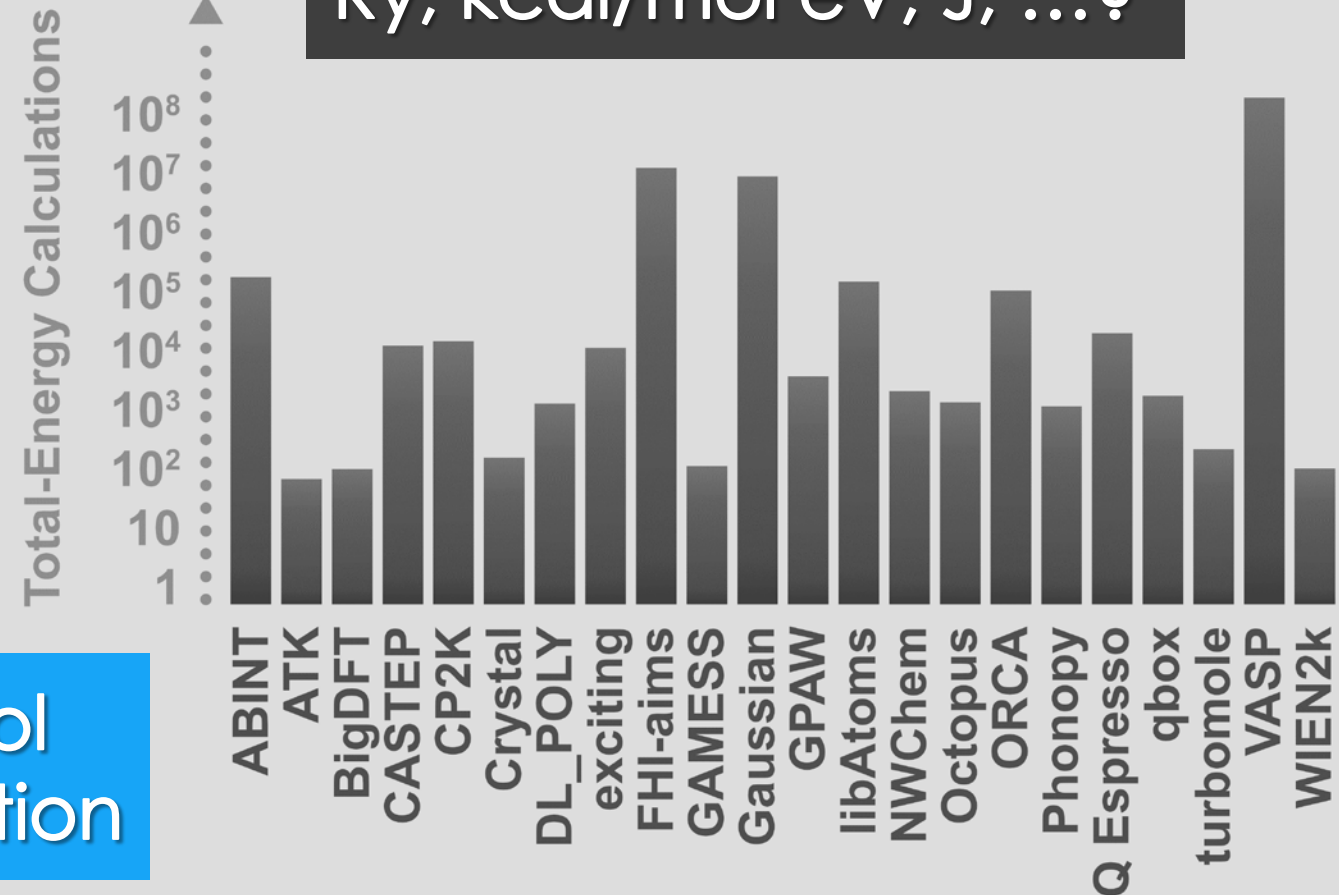
Crucially important

Unique description of data

Every output fully parsed



Ry, kcal/mol eV, J, ...?



Quality control  
Error quantification



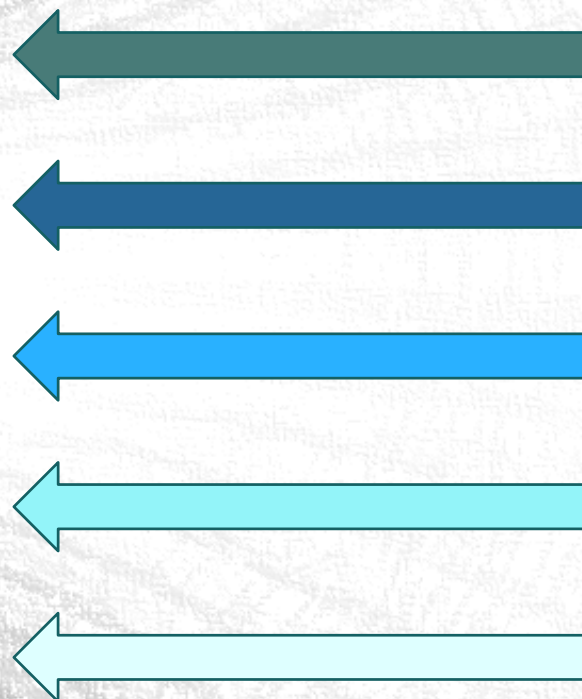
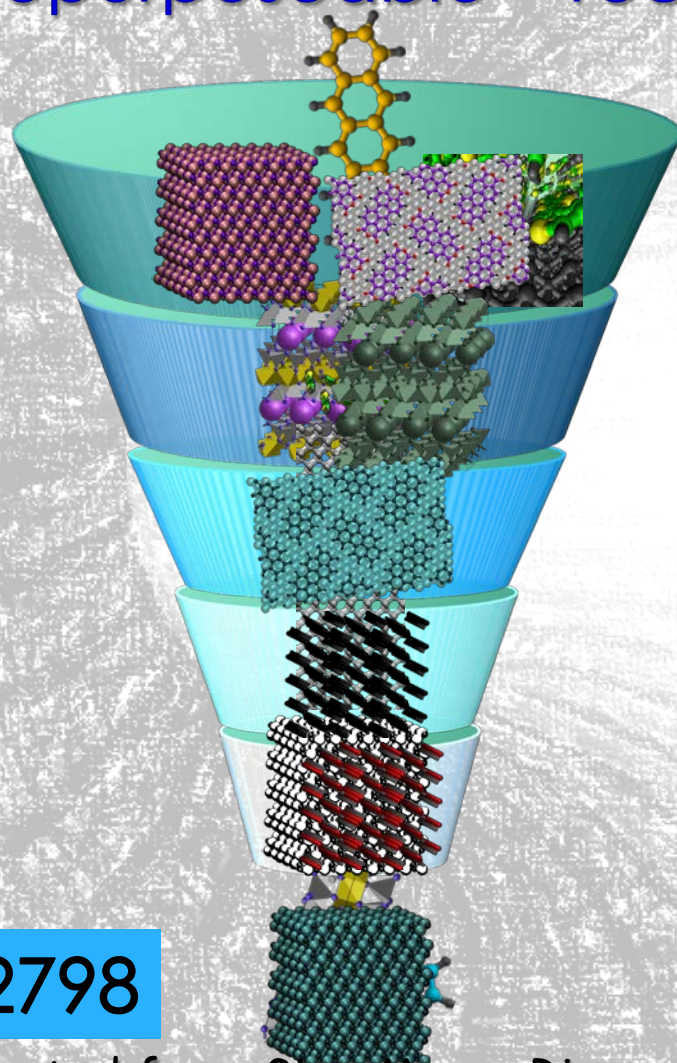
**R**eusable

# High-throughput screening

Reusable = repurposeable = *recyclable*



12798



Property 1

Property 2

Property 3

Property 4

Property 5

3

**N**ext steps ... ..

# From the beginning ...



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FHI Berlin



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HU Berlin



**Claran Clissman**

Pintail Dublin



**Angel Rubio**

MPSD Hamburg



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**Dieter Kranzmüller**

LRZ Munich



**Francesc Illas**

Univ. Barcelona



**Jose Maria Cela**

BSC Barcelona



# Next steps



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

NOMAD is an Implementation Network at



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

# Thanks !!

