



# DAEMON COST Action

Action Chair: **Kevin Rossi** (TU Delft & TU Delft | The Hague, NL)

# Materials and Society



Bronze

Steel

Cement

Plastics

Stone

Iron

Gunpowder

Ammonia

Silicon

# Materials and Society



Bronze

Steel

Cement

Plastics

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Iron

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1820      1850      1900      1950      2000

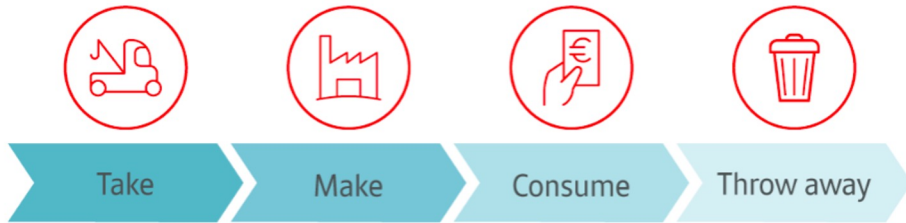
Share not  
In Extreme Poverty

Share In  
Extreme Poverty

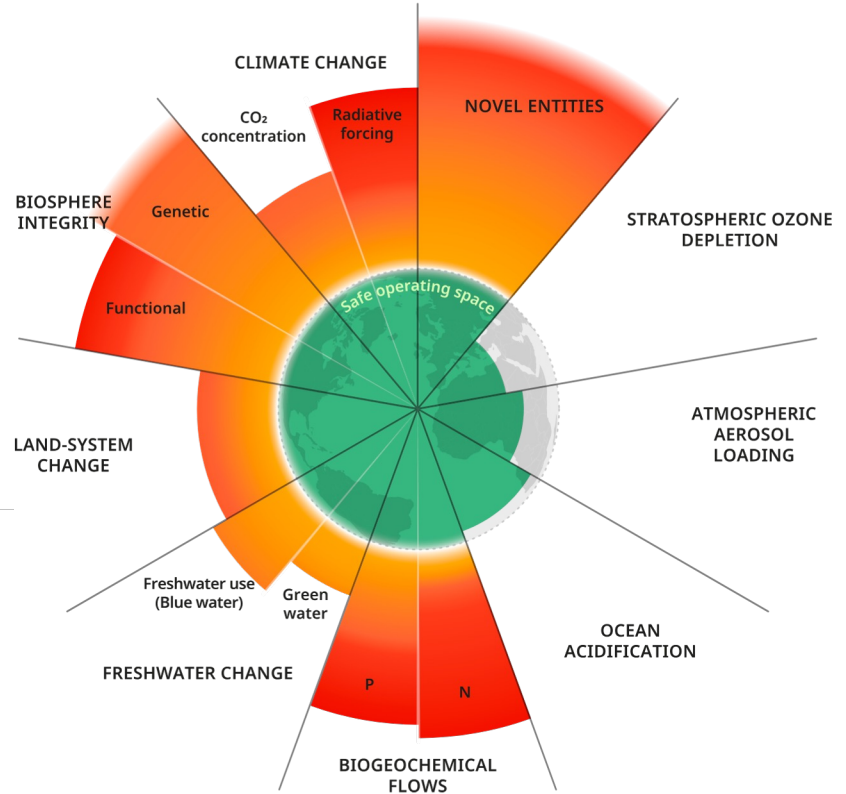
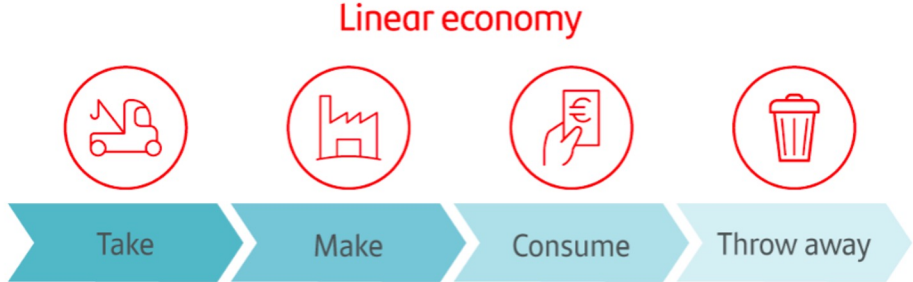
# Materials and Society



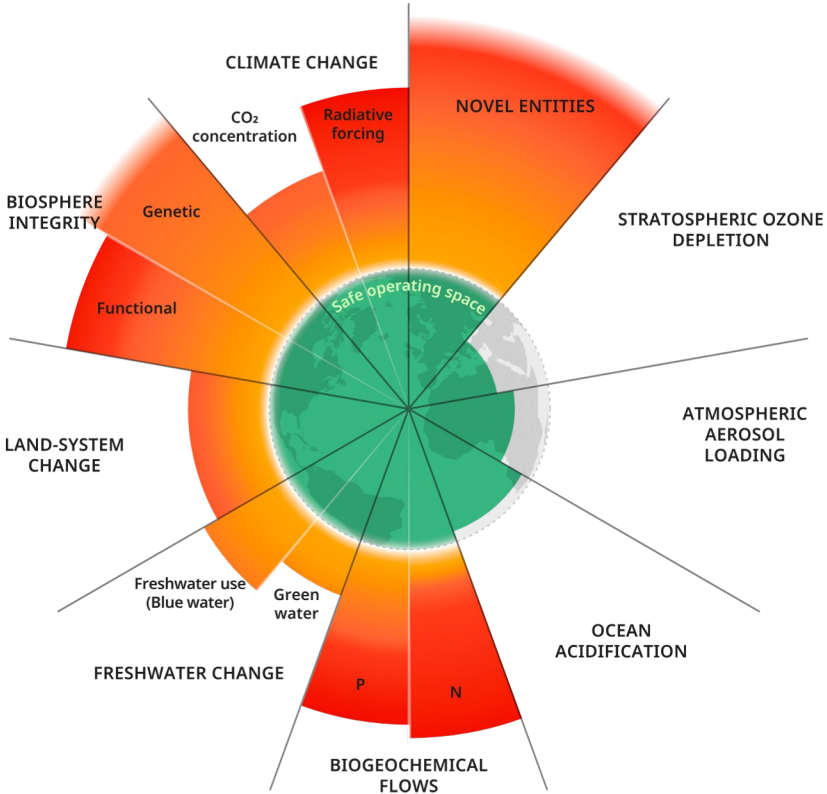
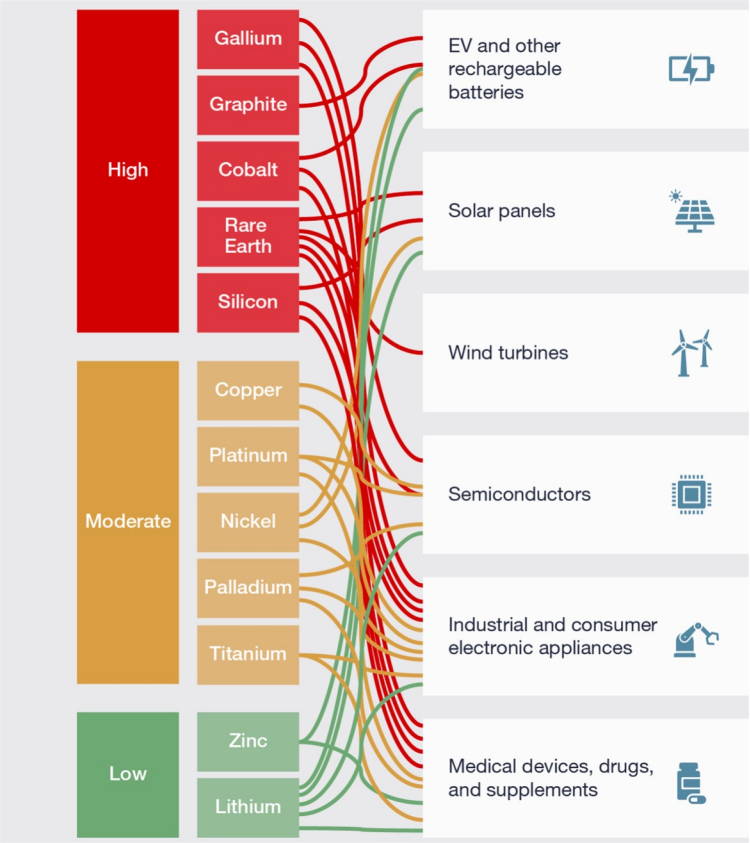
## Linear economy



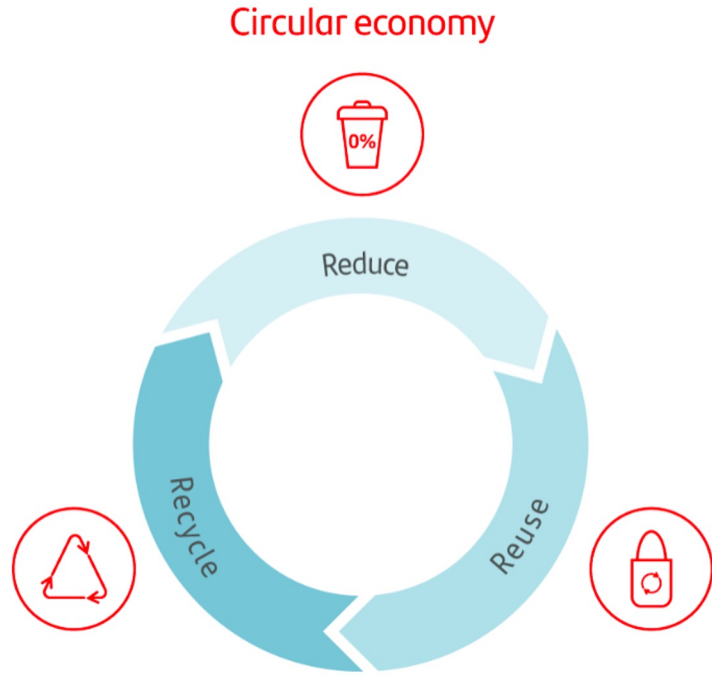
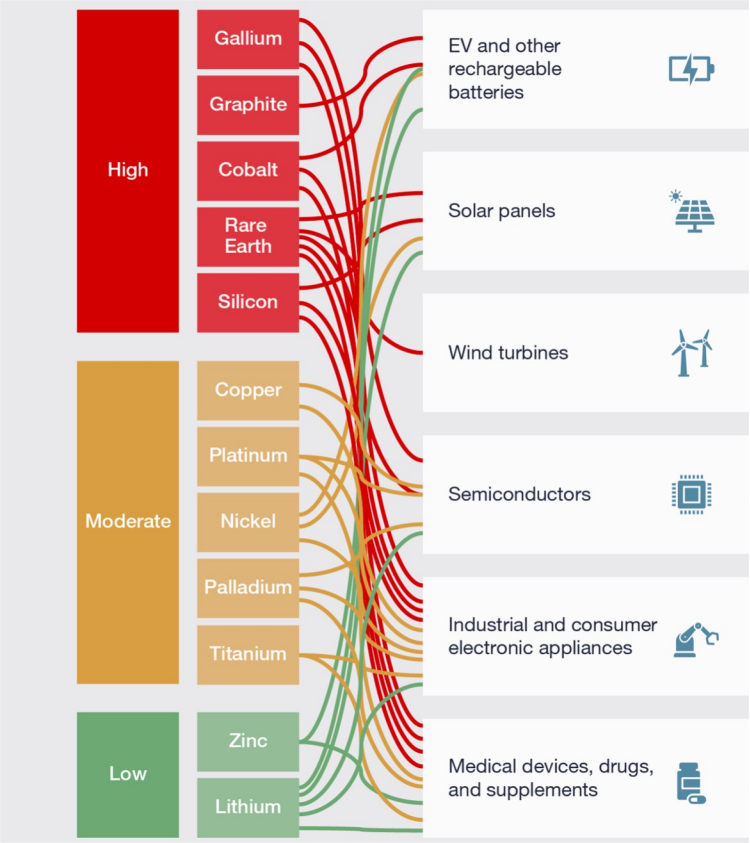
# Materials and Society



# Materials and Society



# Materials and Society



# Materials Science Challenges



***Needle in the  
haystack problem***

*"combinations exceed 65 million for a five-component system ...  
More realistic estimates place the total number of possible materials  
as a googol ( $10^{100}$ )" - Nature Chemistry, 7, 274 (2015)*



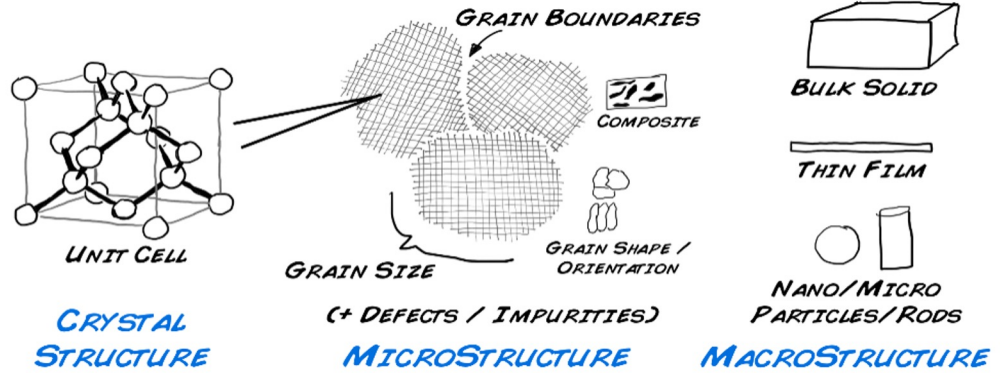
# Materials Science Challenges



*Needle in the haystack problem*

"combinations exceed 65 million for a five-component system ... More realistic estimates place the total number of possible materials as a googol ( $10^{100}$ )" - Nature Chemistry, 7, 274 (2015)

*Multiscale Problem*



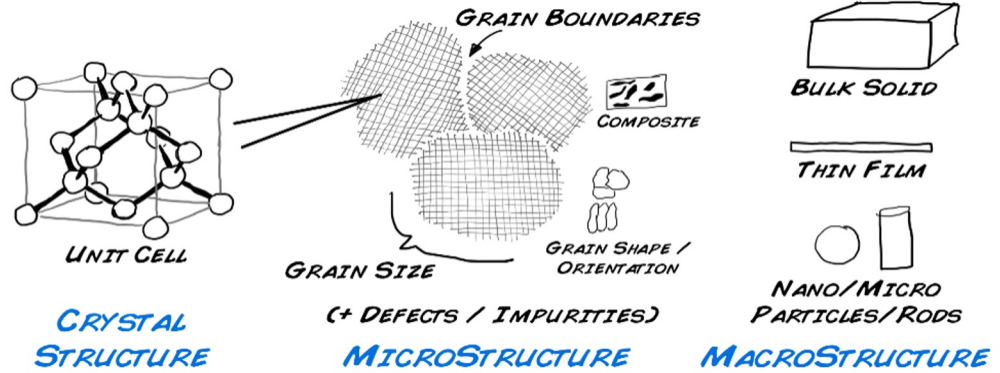
# Materials Science Challenges



Needle in the haystack problem

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Multiscale Problem



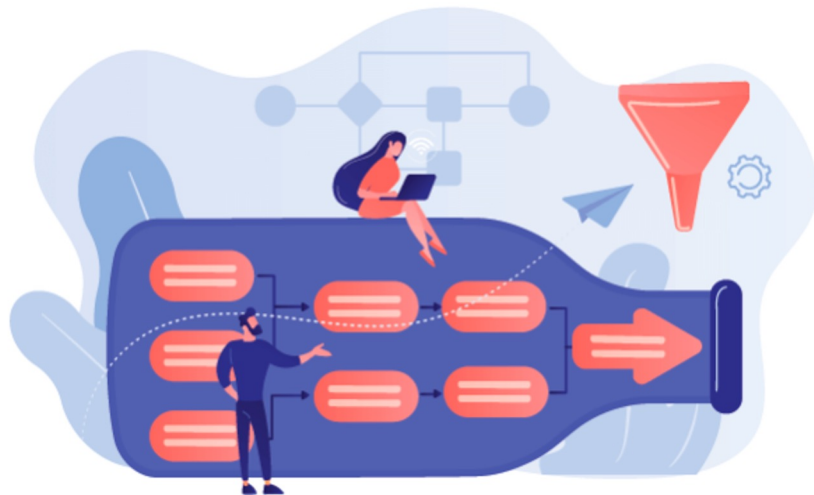
Property-Structure-Processing Complexity



# Digitalising Materials Science



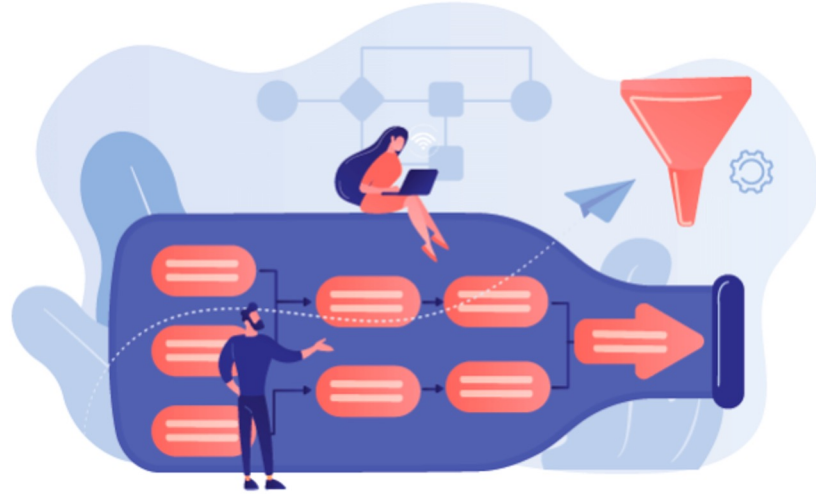
# Digitalising Materials Science



# Digitalising Materials Science



*Efficient and agnostic  
exploration of  
chemical spaces*





*Fast-and-accurate  
approximations of  
complex calculations*

*(Arguably) unbiased  
analysis and discovery*

# Digitalising Materials Science



 UNIVERSITY OF TORONTO |  Acceleration Consortium **Accelerating the discovery of materials and molecules needed for a sustainable future**



Google Brain



Microsoft

Meta



**TOYOTA**  
RESEARCH INSTITUTE



**Schrödinger**



**MAX**

 **NOMAD**  
NOVEL MATERIALS DISCOVERY

 **EoCoE**

# Materials Science Challenges



S&T Excellence				
Grand Challenge: <i>to evolve and accelerate materials discovery strategy</i>				
Challenge (Sec. 1.1.2)	Approach (Sec. 1.2.1)	Coordination Objectives (Sec. 1.2.2)	WGs (Sec. 4)	
<b>C A P A C I T Y</b>	Lack of cross-disciplinary interactions (CiC1)	Foster the creation of a shared language (AiC1)	Harmonise languages, protocols, and data (CBO1) Facilitate exploitation via dissemination (CBO2) Generate/disseminate FAIR DB (RCO1) Promote existing OA codes and models (RCO2)	ALL
	Fragmentation of standards (CiC2)	Facilitate workflows and harmonise frameworks (AiC2)		WG 1
	Competition for talent and gender imbalance (CiC3)	Effective training, mentoring and peer-to-peer networking (AiC3)	Train next-gen researchers (CBO3) Foster diversity, equity, and inclusivity (CBO4)	WG 5
	Unbalanced competitiveness (CiC4)	Efficient methods as level playing field (AiC4)	Facilitate exploitation via dissemination (CBO2) Outreach on digital materials (CBO5) Connect with policymakers and industry (CBO6)	WG 1 WG 5
	Absence of a bridge between Labs and SMEs (CiC5)	Promote two-way interactions between Labs, SMEs and policymakers (AiC5)	Connect with policymakers and industry (CBO6)	WG 4 WG 5

# Materials Science Challenges



S&T Excellence				
Grand Challenge: <i>to evolve and accelerate materials discovery strategy</i>				
Challenge (Sec. 1.1.2)	Approach (Sec. 1.2.1)	Coordination Objectives (Sec. 1.2.2)	WGs (Sec. 4)	
<b>R E S E A R C H</b>	Heterogeneous nature of data (CiR1)	Data-fusion in materials science (AiR1)	Generate/disseminate FAIR databases (RCO1) Multi-modal -objective materials design (RCO6)	
	Inhomogeneous quality of data (CiR2)	Multi-fidelity ML (AiR2)		WG 1 WG 3
	Emulators-real data complexity gaps (CiR3)	Develop new theories (AiR3)	Interdisciplinary approaches and theories (RCO3)	WG 2
	Trustworthy ML domains estimates (CiR4)	ML uncertainty estimation and propagation (AiR4)	Adopt uncertainty-aware ML models (RCO4) Promote existing OA codes and models (RCO2)	WG 2
	Understanding of structure-to-property relationship (CiR5)	Push the methodological boundaries (AiR5)	Interdisciplinary approaches and theories (RCO3) Protocols for materials KPI prediction (RCO5)	WG 2 WG 3 WG 4
	Lack of holistic material design routes (CiR6)	Multiscale multi-objective optimisation algorithms (AiR6)	Protocols for materials KPI prediction (RCO5) Multi-modal and objective design (RCO6)	WG 3 WG 4



# What's a COST Action ?



## Excellence and inclusiveness

### COST Member Countries

#### 41 COST Members

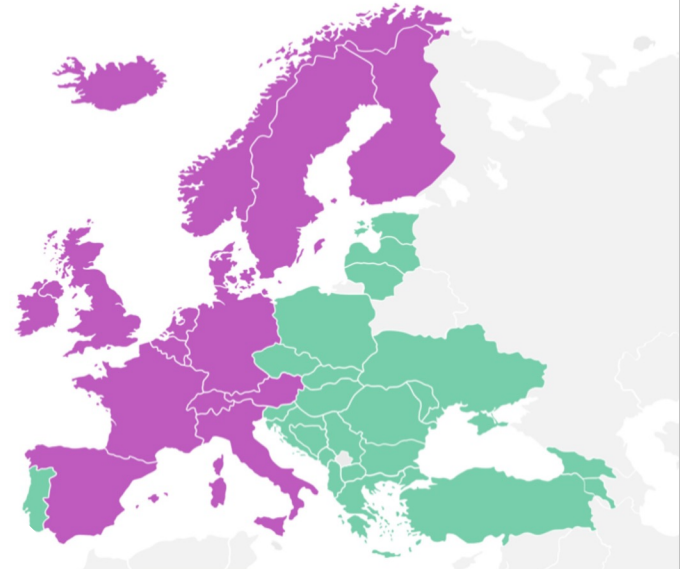
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#### 1 Cooperating Member

- Israel

#### 1 Partner Member

- South Africa



# DAEMON COST



**WG1:** Community standards: data, workflows and codes for materials design.

**WG2:** Representations and algorithms for materials design for “single-modality” use.

**WG3:** Multi-modal machine learning methods for advanced materials design.

**WG4:** Process-structure-property relationships in materials. Novel insights and applications.

**WG5:** Training, Dissemination, Exploitation, Outreach

# DAEMON - 05-06/02/2024



60+ Participants from Academia  
30+ Countries represented



Industrial Leaders, start-ups, & Investors  
in green energy and sustainable chemistry







# DAEMON - 13-17/05/2024



## Machine Learning Modalities for Materials Science

Jožef Stefan Institute, Ljubljana, Slovenia



Language Models &  
Text Mining



Multi-modal  
Machine Learning



Computer  
Vision



Multi-fidelity  
Machine Learning



Symmetry

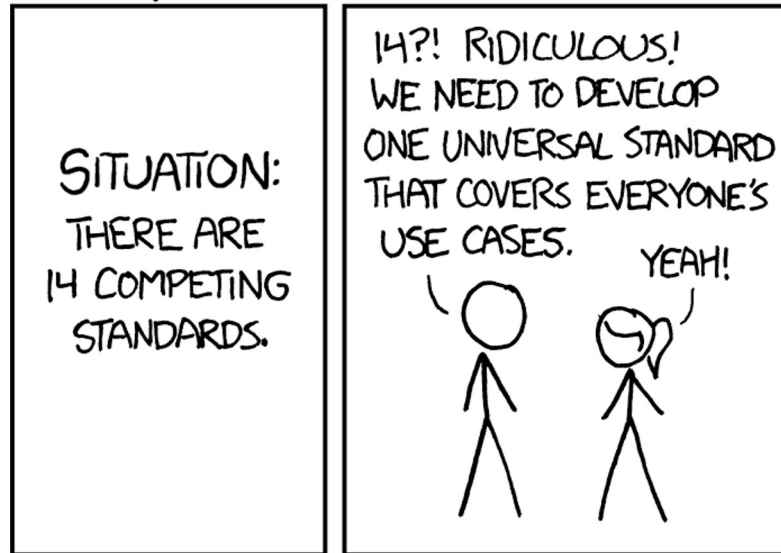


Conservation laws

Physics-Based  
Machine Learning

## Standards, FAIR Data, & Open-Science

HOW STANDARDS PROLIFERATE:  
(SEE: A/C CHARGERS, CHARACTER ENCODINGS, INSTANT MESSAGING, ETC.)



# Growing a DAEMON



## Standards, FAIR Data, & Open-Science

HOW STANDARDS PROLIFERATE:  
(SEE: A/C CHARGERS, CHARACTER ENCODINGS, INSTANT MESSAGING, ETC.)

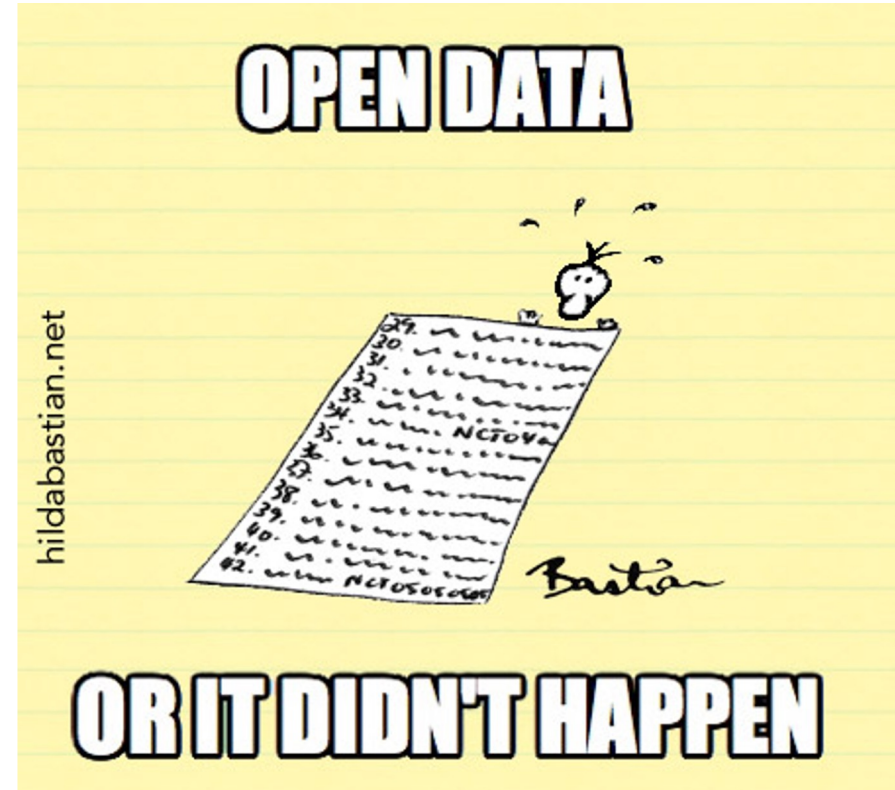




# Standards – in publishing



Standards,  
FAIR Data, &  
Open-Science





## **Machine learning in scanning transmission electron microscopy**

**nature reviews** methods primers


## **Machine learning for analysis of experimental scattering and spectroscopy data in materials chemistry**

**Chemical Science**



**Open-science,  
a matter of  
policy**

## NWO DMP assessment rubric

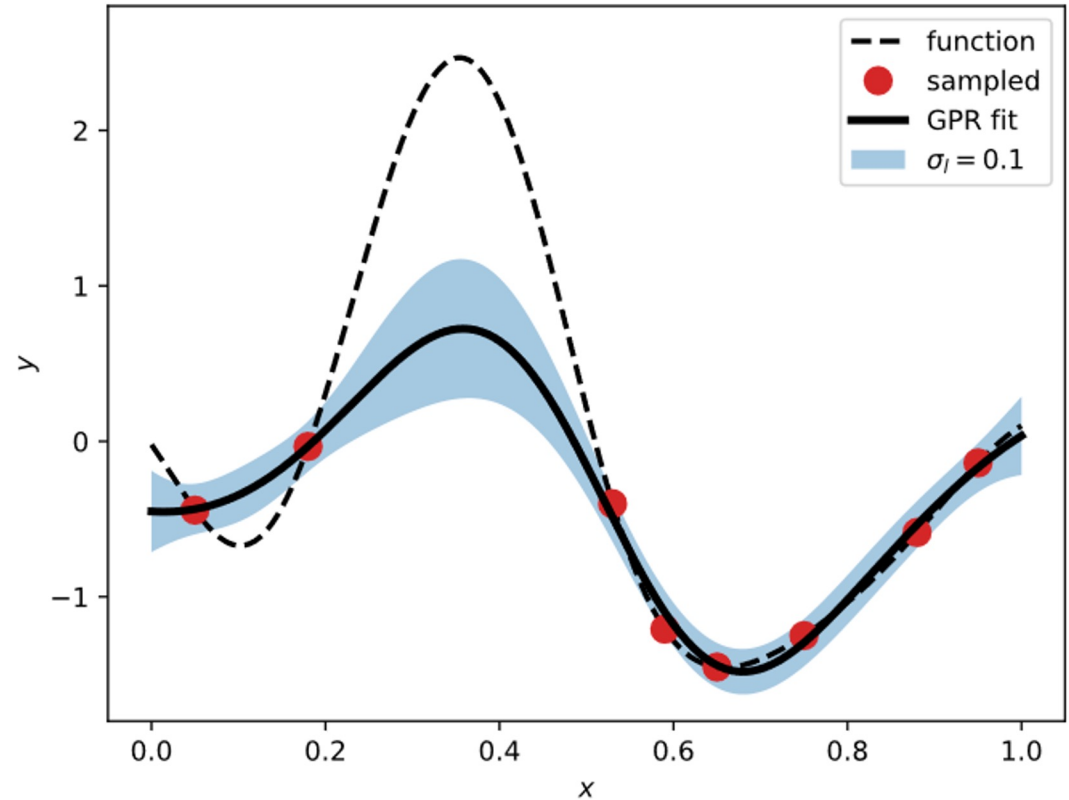
Cruz, Maria<sup>1</sup> ; van den Berg, Eveline<sup>1</sup> 



# Growing a DAEMON



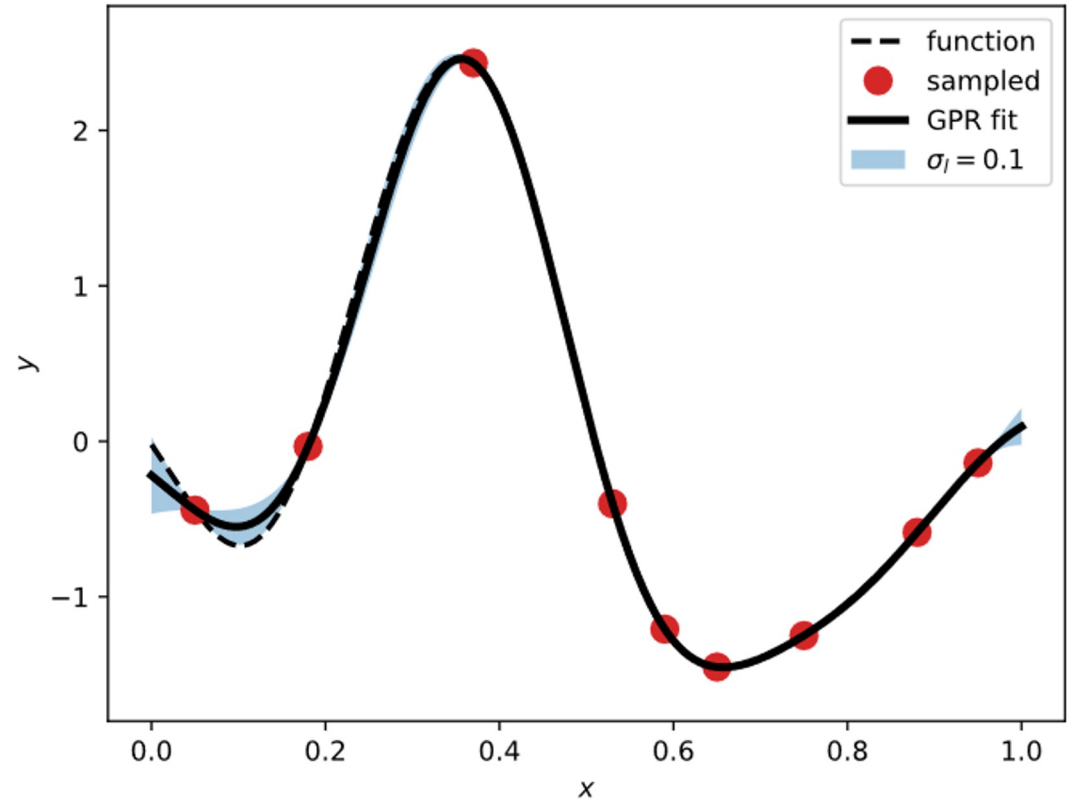
Reliable and  
trustworthy  
predictions



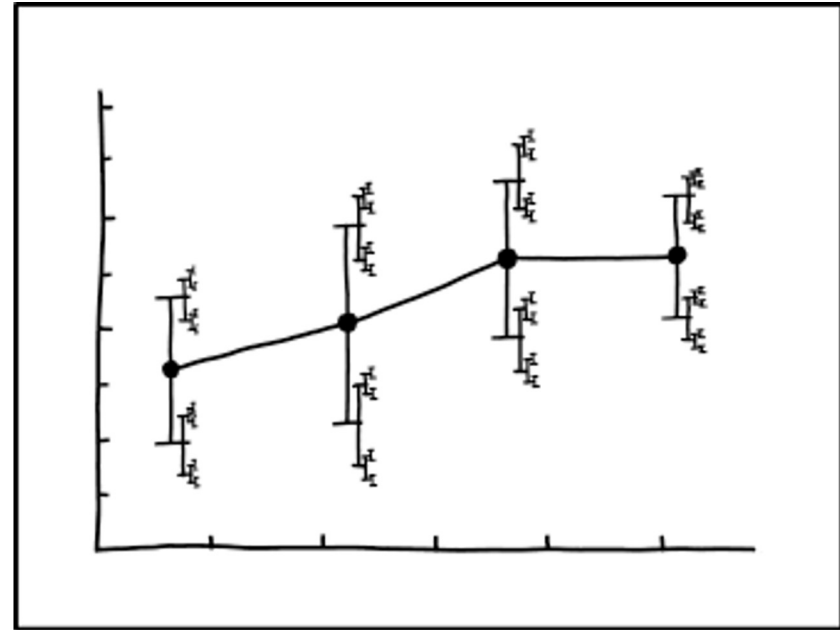
# Growing a DAEMON



Reliable and  
trustworthy  
predictions



## Uncertainty review

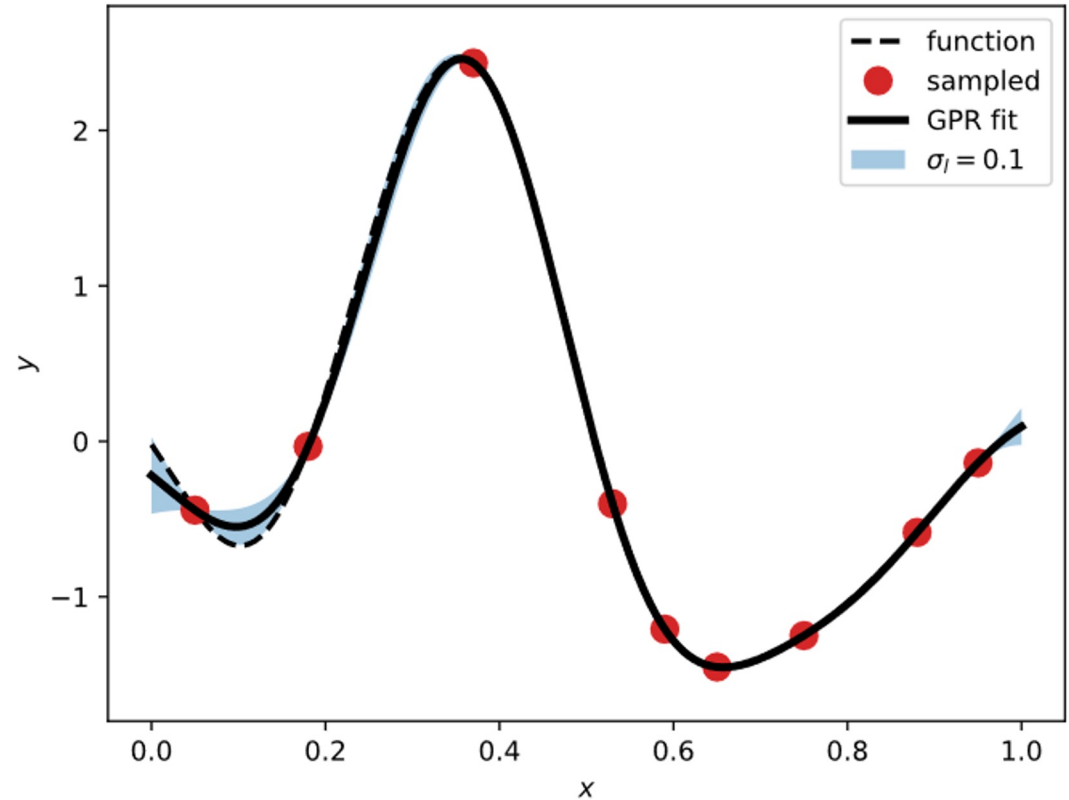


I DON'T KNOW HOW TO PROPAGATE  
ERROR CORRECTLY, SO I JUST PUT  
ERROR BARS ON ALL MY ERROR BARS.

# Growing a DAEMON



Reliable and  
trustworthy  
predictions



# Growing a DAEMON



Training new  
generations





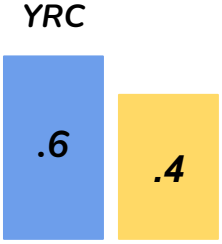
# DAEMON-graphics



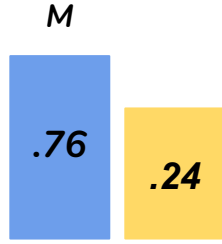
*Initial Proposers*



*Countries Represented*



*Career Stage*



*Gender Balance*

# DAEMON-graphics



**Initial Proposers**



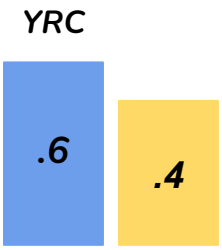
**Countries Represented**



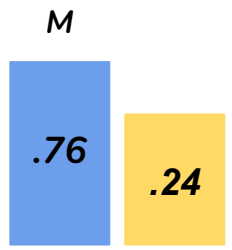
**Affiliated Members**



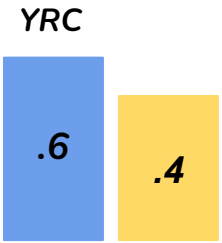
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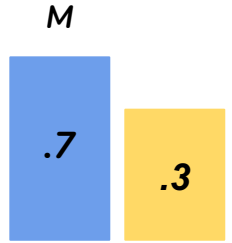
**Career Stage**



**Gender Balance**



**Career Stage**



**Gender Balance**

# DAEMON-graphics



# COST Activities

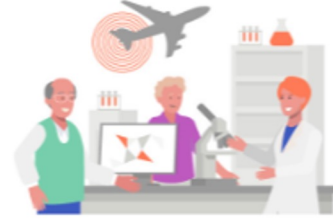


**Budget:** ~600K EUR over 4 years

**Objective:** Build capacity and foster research coordination



Organising meetings,  
workshops & conferences



Short-term scientific  
missions



Training schools



Communication  
& dissemination activities



Virtual  
networking tools

# Scientific Missions



**Purpose:** Training and exchange of knowledge.  
Fostering collaboration on a specific scientific question.  
Facilitate breakthroughs and increase technological impact.





**Purpose:** supporting young researchers (<40 years old) and students in IT Countries and NN Countries to attend events not organized by the COST Action related to, but not organized by, the Action.

## COST Member Countries

### 41 COST Members

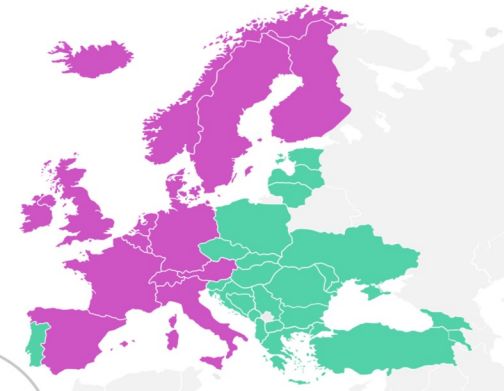
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- COST Members
- COST Members ITCs
- COST Cooperating Member
- COST Partner Member
- Other Countries

# Internal guide - Open Calls



Internal guide: [https://cost-daemon.eu/?page\\_id=180](https://cost-daemon.eu/?page_id=180)

A screenshot of the DAEMON website homepage. The background is dark grey with a pattern of white circles and lines. On the left, there is a large white 'DAEMON' logo. In the center, the text 'DAEMON - COST' is displayed in large white letters. Below it, the tagline 'Data-driven applications towards the engineering of functional materials' is visible. At the top right, a navigation menu is open, showing options like 'Job Listings', 'Open Calls', 'Short-Term Scientific Mission Grant', 'ITC Conference Grant', and 'Dissemination Grant'. The 'Open Calls' option is highlighted with a blue arrow.

Home News Events ▾ Opportunities ▾ Structure ▾ Join us! Privacy

Job Listings

Open Calls >

Short-Term Scientific Mission Grant

ITC Conference Grant

Dissemination Grant

**DAEMON – COST**

Data-driven applications towards the engineering of functional materials



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