



Leibniz ScienceCampus  
**Digital Transformation  
of Research**

**Interdisciplinary Colloquium on Digitalisation of Research  
Leibniz Science Campus "Digital Transformation of Research" (DiTraRe)**

# **AI for Materials Science - From Autonomous Materials Optimization to the Generation of Novel Ideas**

*Pascal Friederich*

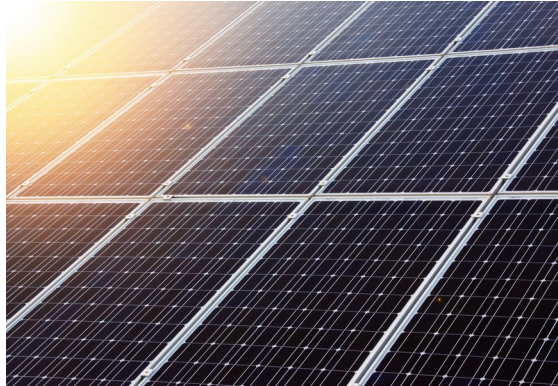
**Email:** [pascal.friederich@kit.edu](mailto:pascal.friederich@kit.edu)

**Web:** [aimat.science](http://aimat.science)

**2 July 2026**

# Materials are the driver for innovation

**Renewable energy**  
**Photovoltaics**  
**Batteries**



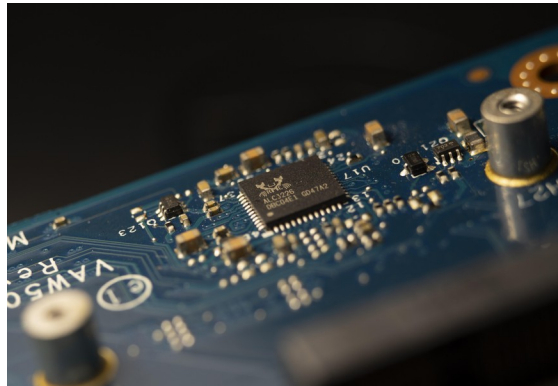
By PublicDomainPictures via Pixabay



By padrinan via Pixabay

**Medicine**  
**Antibiotics**  
**Vaccines**

**Electronics**  
**Chips**  
**Semiconductors**



By Henryphoto via Pixabay



By LPArT via Pixabay

**Mobility**  
**Transport**  
**Aerospace**

## Critical contributions of materials research

- **Clean-energy** materials (batteries, solar cells, magnets)
- **Environment-friendly** construction materials
- **Non-toxic** replacements of base chemicals
- Materials for innovative **health** technologies
- **Sustainable** production and processing



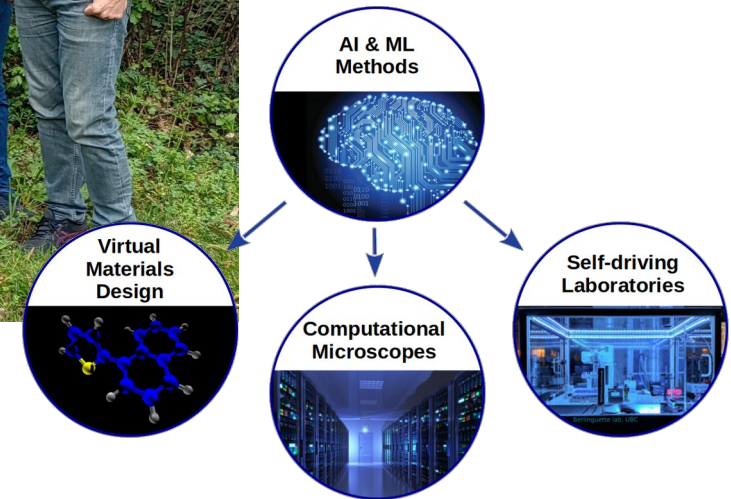
<https://sdgs.un.org/goals>

# Research group AI for Materials Science (AiMat)

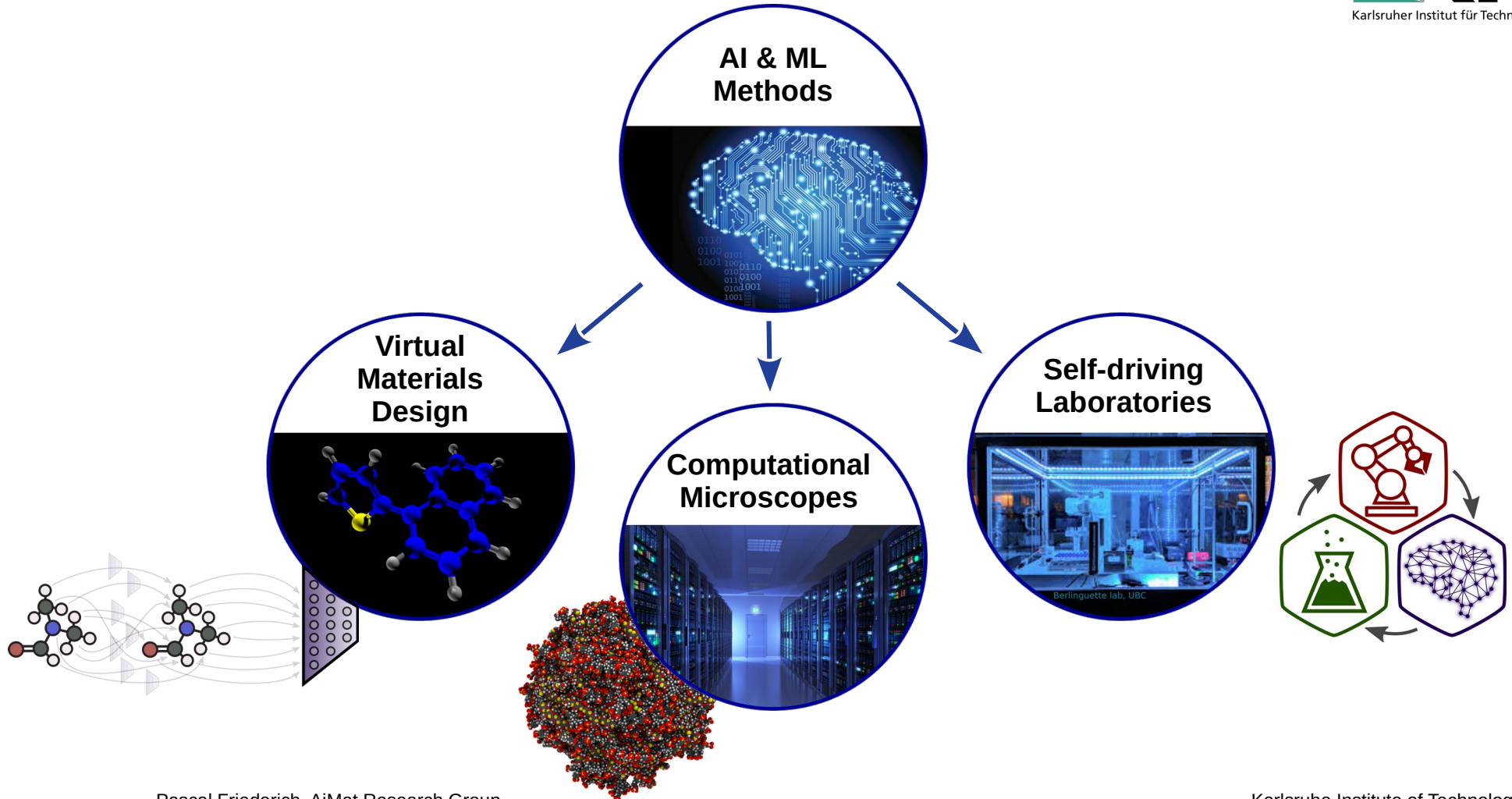


**Bridge between**

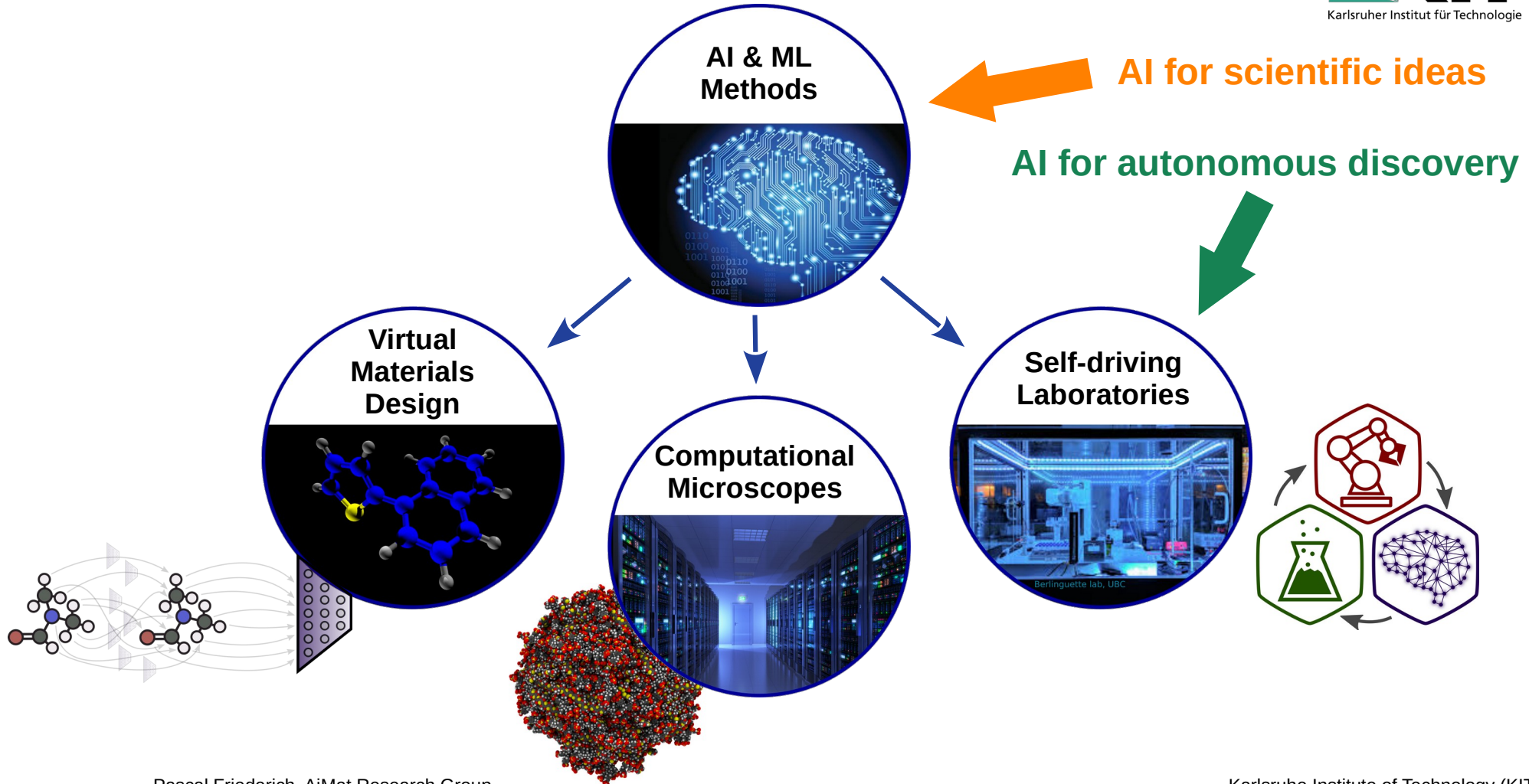
- **Methods development in computer science**
- **Applications in materials science and chemistry**



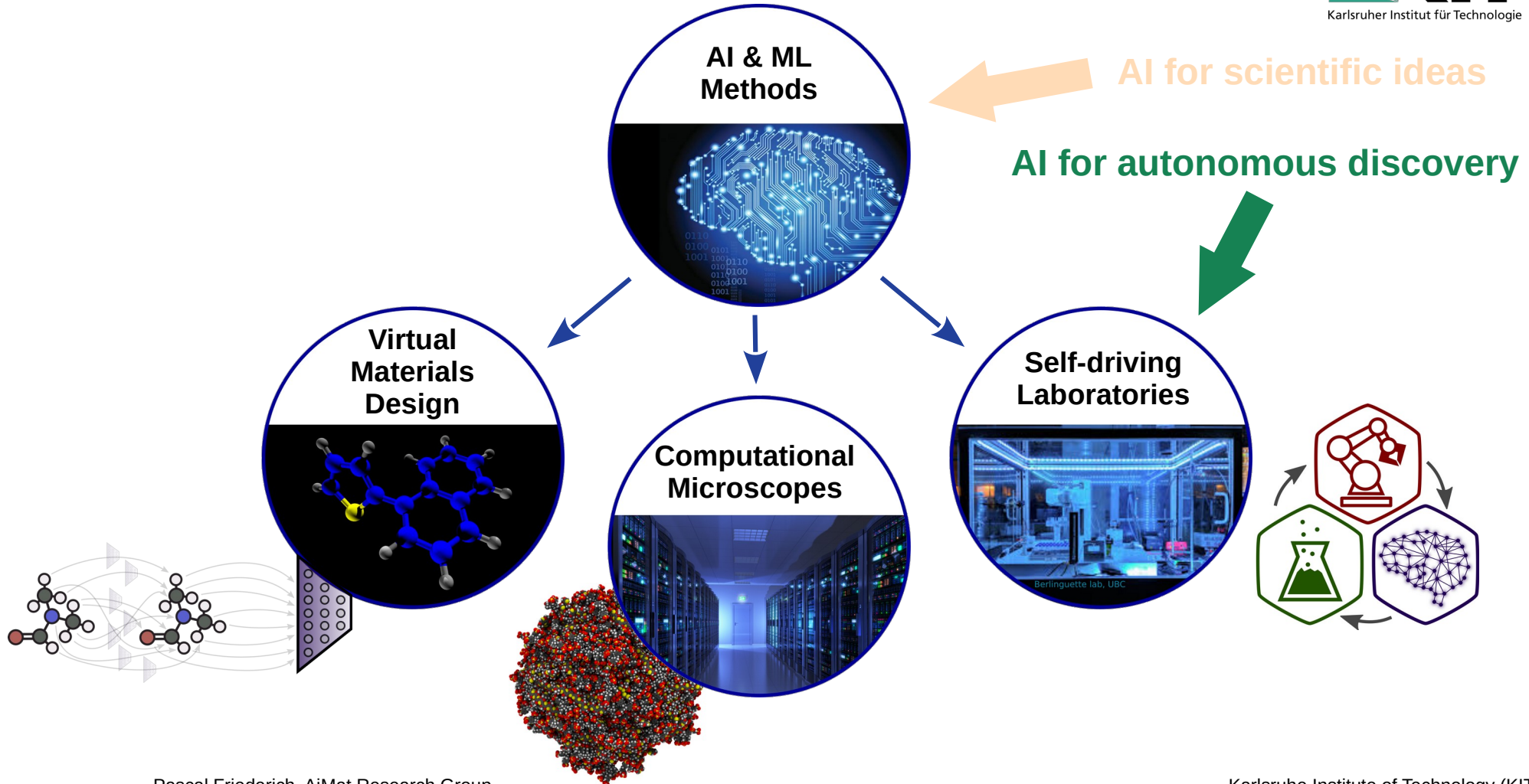
# Machine Learning for Materials Science and Chemistry



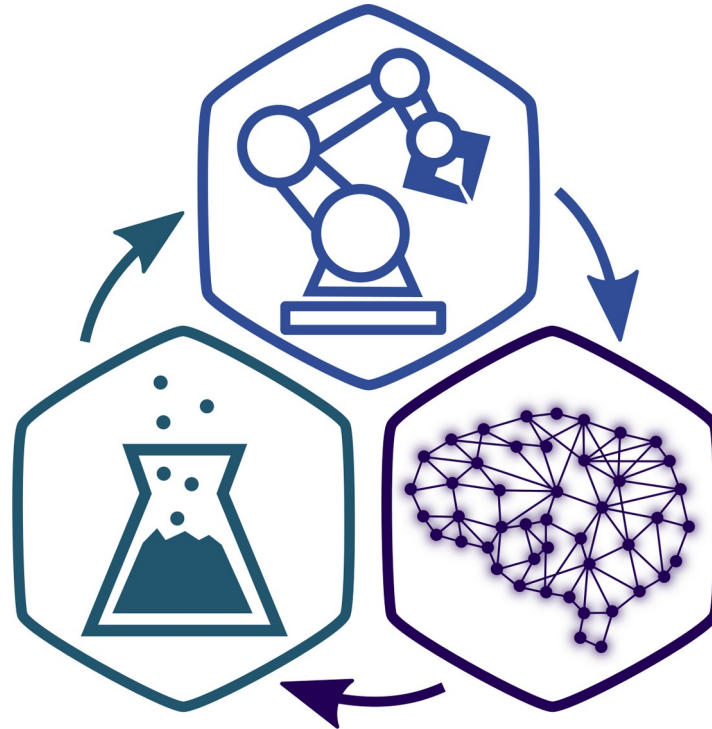
# Machine Learning for Materials Science and Chemistry



# Machine Learning for Materials Science and Chemistry



Idea

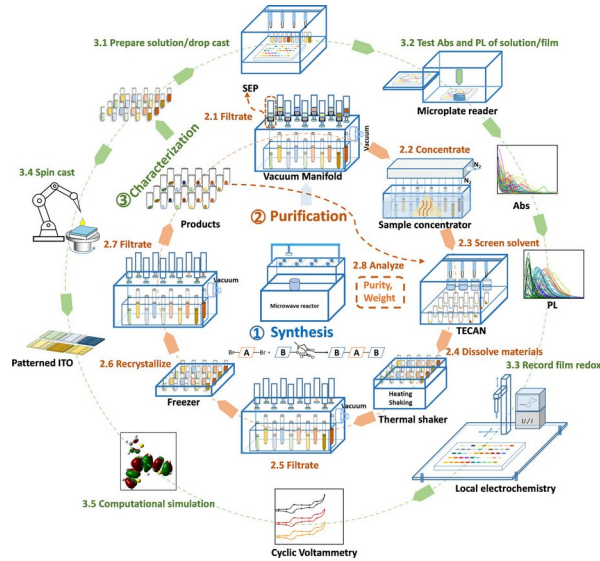


Closing the loop



# Design of solar cell materials

From synthesis ...



...to devices!



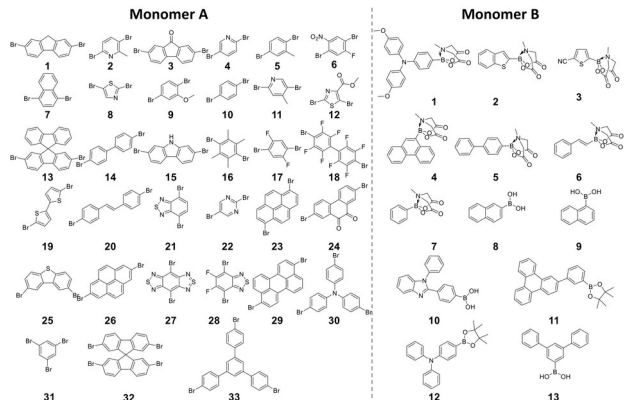
10.1021/acs.accounts.4c00095



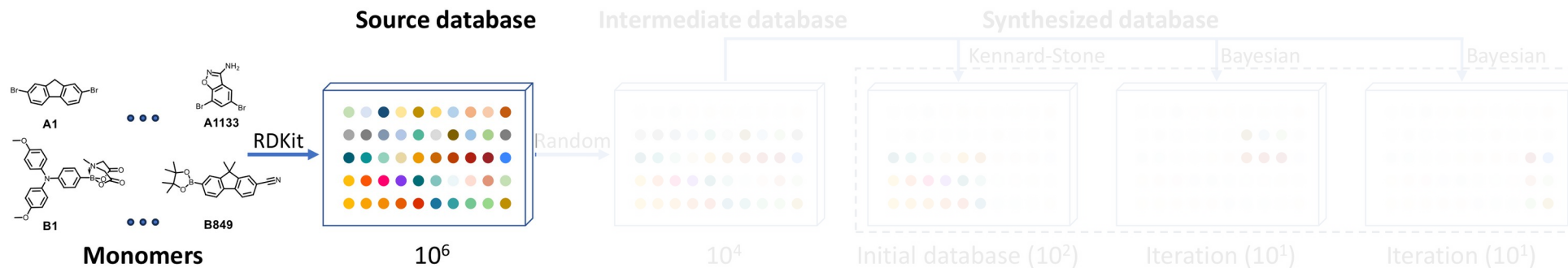
Christoph  
Brabec

Wu, Friederich, Brabec *et al.*, JACS, **2023**.  
Wu, Friederich, Brabec *et al.*, Science, **2024**.

# Synthesis in a space of 1,000,000 molecules

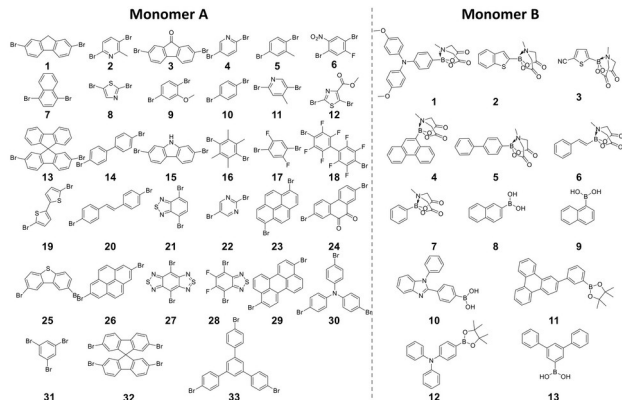


- Hole transport materials for **perovskite solar cells**
  - Automated synthesis of A-B-A molecules
  - Library of ~1000 A and ~1000 B fragments
- **Chemical space of 1,000,000 molecules**



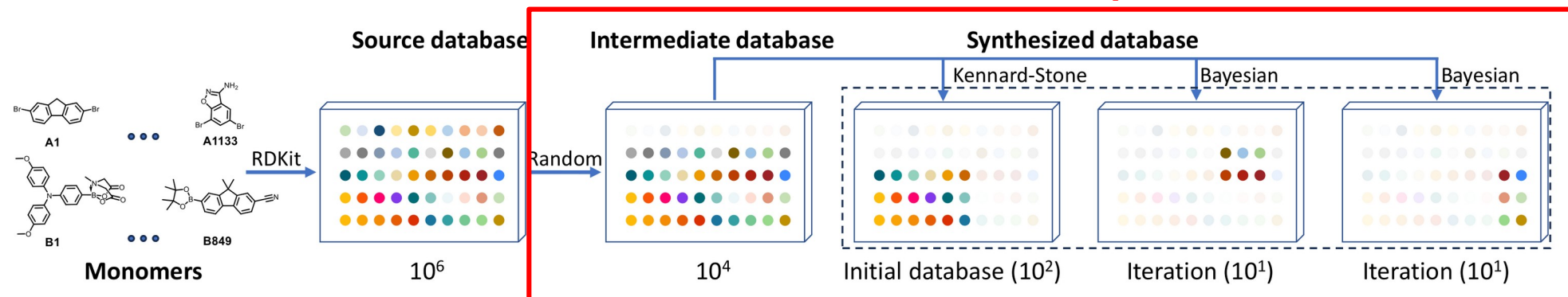
Wu, Friederich, Brabec *et al.*, JACS, **2023**.  
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# Synthesis in a space of 1,000,000 molecules



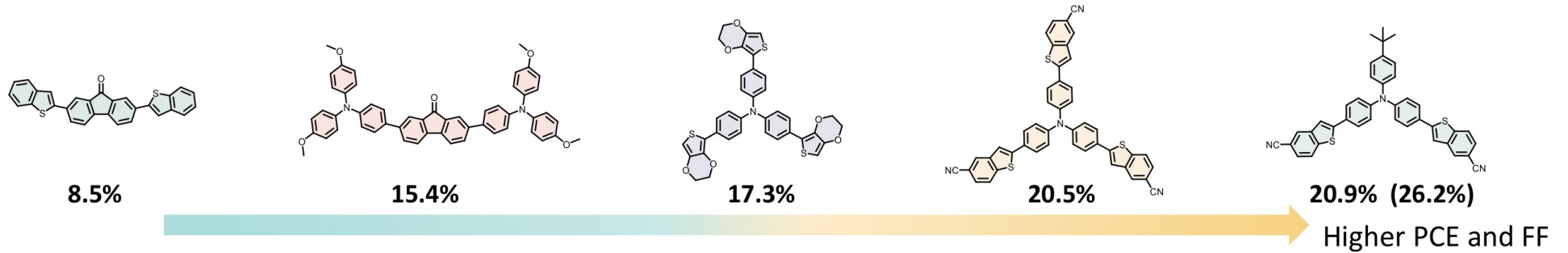
- Hole transport materials for **perovskite solar cells**
- Automated synthesis of A-B-A molecules
- Library of ~1000 A and ~1000 B fragments  
→ **Chemical space of 1,000,000 molecules**

## Autonomous exploration



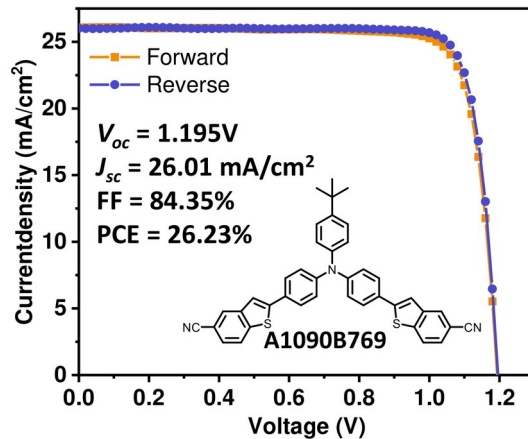
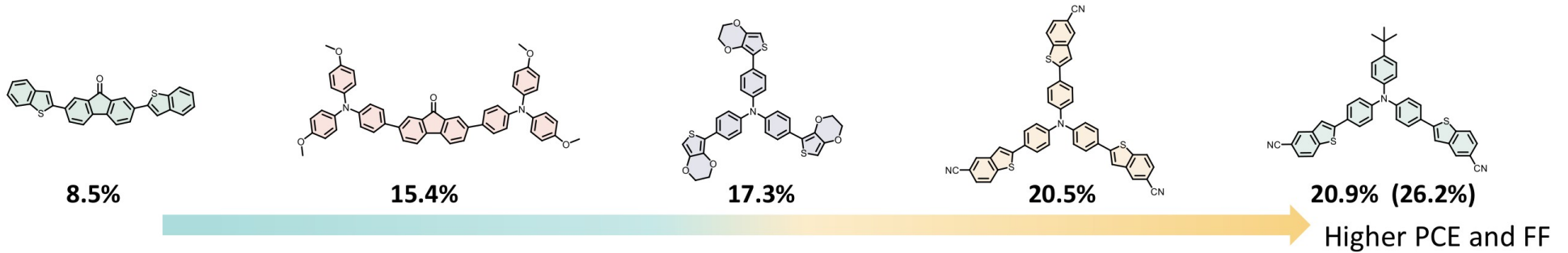
Wu, Friederich, Brabec *et al.*, JACS, **2023**.  
Wu, Friederich, Brabec *et al.*, Science, **2024**.

# Optimization of device performance through HTL design



Wu, Friederich, Brabec *et al.*, JACS, **2023**.  
Wu, Friederich, Brabec *et al.*, Science, **2024**.

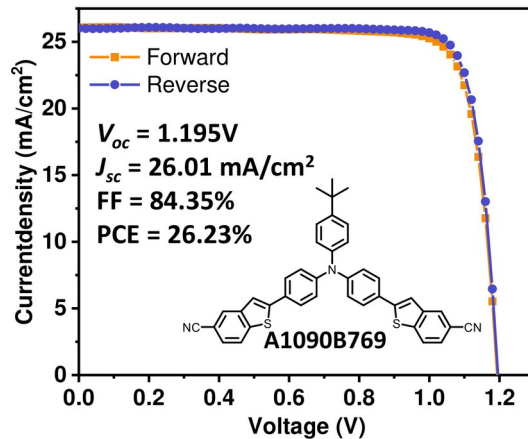
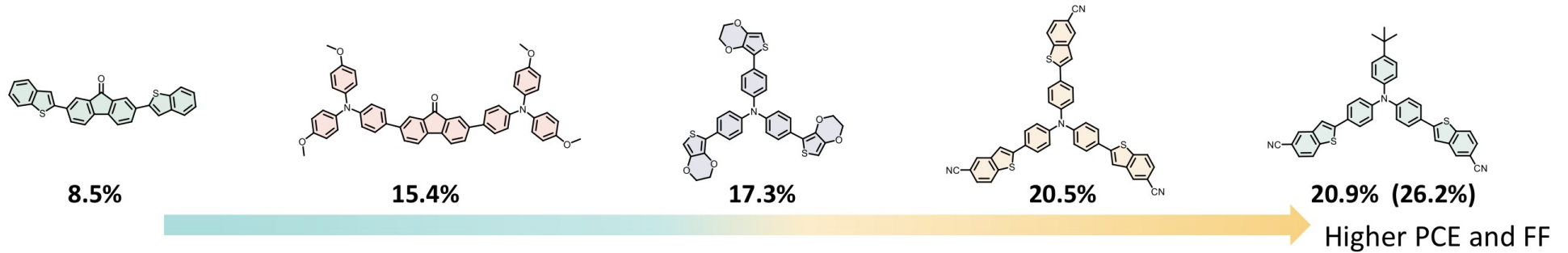
# Optimization of device performance through HTL design



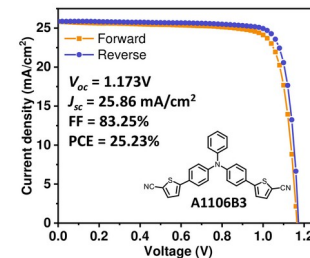
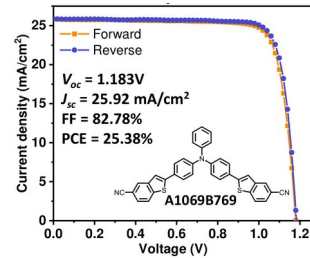
Performance in optimized device: 26.2%

Wu, Friederich, Brabec *et al.*, JACS, 2023.  
Wu, Friederich, Brabec *et al.*, Science, 2024.

# Optimization of device performance through HTL design



## Multiple candidates with >25% efficiency!



Wu, Friederich, Brabec *et al.*, JACS, 2023.  
Wu, Friederich, Brabec *et al.*, Science, 2024.

# HELMA HELMHOLTZ Acceleration Alliance

Think Bigger and Faster:  
The Helmholtz Acceleration Alliance

```
mirror_ob.select = 1  
modifier_ob.select = 1  
mirror_ob.use_x = False  
mirror_ob.use_y = False  
mirror_ob.use_z = True  
bpy.context.scene.objects.active = modifier_ob  
print("Selected" + str(modifier_ob)) # modifier ob is the active ob
```

## Decentralized Self Driving Lab Network

### Health Technologies (HealthTech)

### Accelerated & Autonomous Material Discovery (A2MD)



<b>Biomaterials for Bioprinting</b>	<b>Drug Discovery</b>	<b>Tissues &amp; Organoids</b>	<b>Multomics/ Spatial</b>	<b>Bio-Carriers</b>	<b>Bio-Factories</b>	<b>Smart Implants</b>	<b>Bio-Materials</b>	<b>Polymers</b>	<b>Molecular Imaging</b>	<b>High-Entropy &amp; Cluster-Based Mat.</b>	<b>Catalysis</b>	<b>High-Throughput Analytics</b>	<b>High-Throughput Discovery</b>	<b>Energy Conversion</b>	<b>Circular Materials</b>	<b>Sustainable Organic Substitutes</b>
<b>Bio-electronics Sensors</b>	<b>Bio-coatings</b>	<b>Bio-analytics</b>	<b>Bio-NMR</b>	<b>Micro machines</b>	<b>Bio-processing</b>	<b>Implant Corrosion</b>	<b>In situ Analytics</b>	<b>Automated Cell Culture</b>	<b>Proteomics</b>	<b>Smart Electronics</b>	<b>Energy Storage</b>	<b>Photonics</b>	<b>Sustainable Light Conversion</b>	<b>Photo-voltaics</b>	<b>Emerging Opto-electronics</b>	<b>Emerging Electronics</b>

Helmholtz Biomedical Engineering

Partners from Helmholtz Health

Partners from Helmholtz Energy

### Tech Lab

<b>Robotics</b>	<b>Automation</b>	<b>Miniaturization</b>	<b>Micro-fluidics</b>	<b>Synthetic Biology</b>	<b>Synthesis</b>
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### Pioneer Campus

<b>Innovation</b>	<b>Pioneer Campus</b>	<b>Think Tank</b>	<b>Life Long Learning</b>	<b>Research Oriented</b>
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### AI Lab

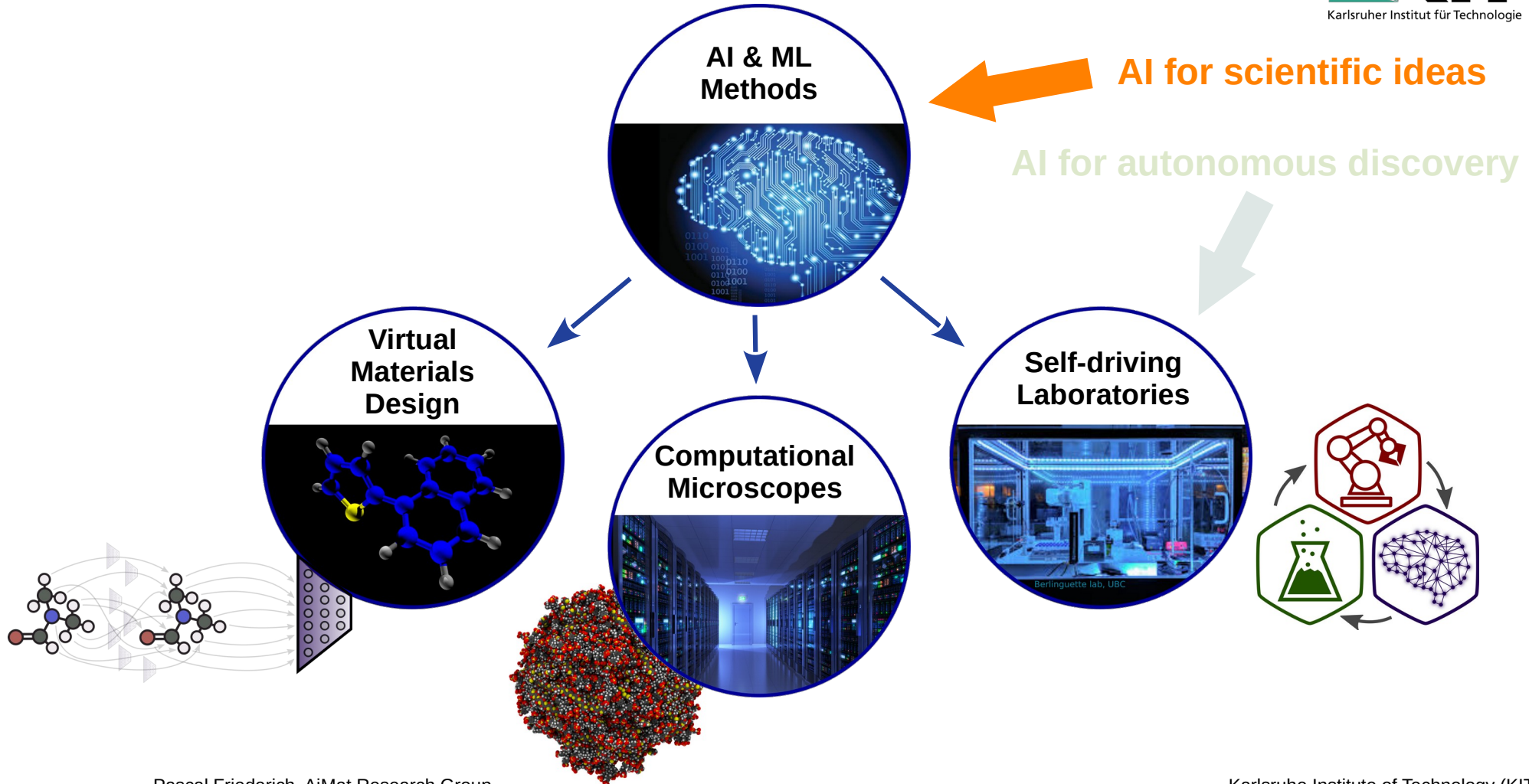
<b>AI &amp; Machine Learning</b>	<b>Digital Twins</b>	<b>ELN</b>	<b>First Principles Theory</b>	<b>Simulation</b>
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HELMHOLTZ QUANTUM

### Outreach

<b>Living Lab „AI in Health“</b>	<b>Hands-on Laboratory</b>	<b>Maker Space</b>	<b>Open Discussion Plattform</b>	<b>Lecture Series</b>	<b>Public Outreach</b>	<b>Social Media</b>	<b>Digital Outreach</b>
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# Machine Learning for Materials Science and Chemistry



# Scientific progress

Scientific  
knowledge

KNOWN  
KNOWNS

“things that we’re  
aware that we know”

KNOWN  
UNKNOWNNS

“things that we’re  
aware that we **don’t** know”

Scientific  
creativity

Scientific  
intuition

UNKNOWN  
KNOWNS

“things that we’re  
**unaware** that we know”

UNKNOWN  
UNKNOWNNS

“things that we’re **unaware**  
of and **don’t** know”

Serendipity,  
random  
discoveries



Image: Doug Belshaw, CC0, <https://blog.dougbelshaw.com/solving-complexity>  
Wikimedia Commons, <https://de.wikipedia.org/wiki/Datei:Iceberg.jpg>

# Scientific progress

Scientific  
knowledge

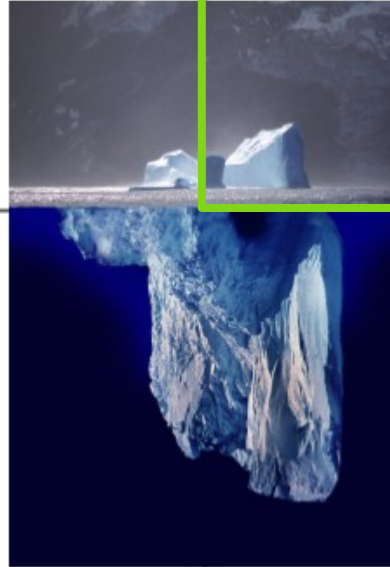
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“things that we’re  
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Scientific  
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UNKNOWN  
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“things that we’re **unaware**  
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Scientific  
creativity

Serendipity,  
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discoveries

Image: Doug Belshaw, CC0

# Creation of scientific ideas



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“things that we’re aware that we know”



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UNKNOWN  
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“things that we’re **unaware** of and **don’t** know”

Image: Doug Belshaw, CC0

# Creation of scientific ideas

Improving an  
existing concept

*Incremental*



**Creativity if ideas**

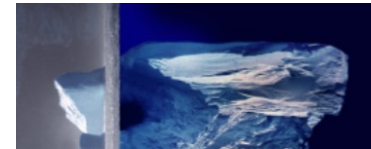
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**UNKNOWN  
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“things that we’re **unaware**  
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Image: Doug Belshaw, CC0

# Creation of scientific ideas

Improving an  
existing concept

Bringing  
concepts  
together

*Incremental*

*Unconventional*



**Creativity of ideas**

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Image: Doug Belshaw, CC0

# Creation of scientific ideas

Improving an  
existing concept

Bringing  
concepts  
together

Introducing  
new concepts

*Incremental*

*Unconventional*

*Disruptive*



**Creativity of ideas**

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“things that we’re  
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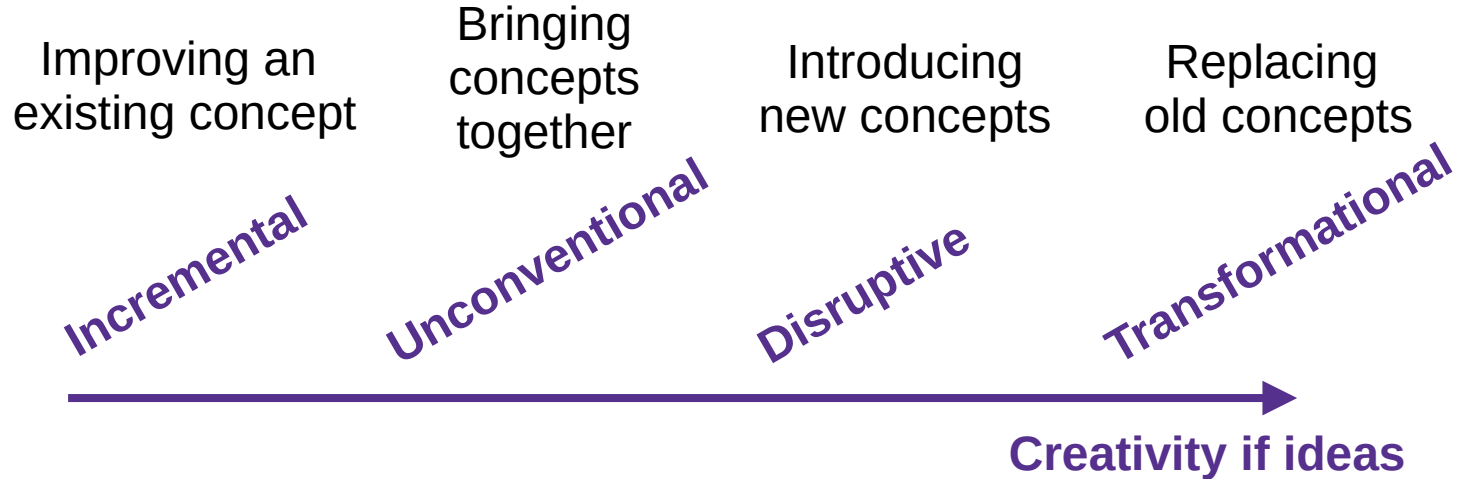


**UNKNOWN  
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“things that we’re **unaware**  
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Image: Doug Belshaw, CC0

# Creation of scientific ideas



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Image: Doug Belshaw, CC0

# Creation of scientific ideas

## LLMs today

Improving an  
existing concept

Bringing  
concepts  
together

Introducing  
new concepts

Replacing  
old concepts

Incremental

Unconventional

Disruptive

Transformational



Creativity of ideas

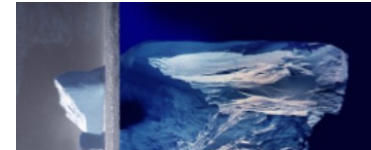
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UNKNOWN  
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“things that we’re **unaware**  
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Image: Doug Belshaw, CC0

# Creation of scientific ideas

## LLMs today

Improving an existing concept

Incremental

Bringing concepts together

Unconventional

## Observations required

Introducing new concepts

Disruptive

Replacing old concepts

Transformational



Creativity of ideas

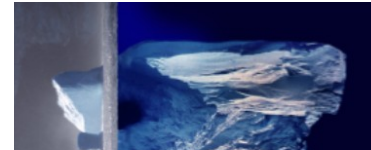
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Image: Doug Belshaw, CC0

# Creation of scientific ideas

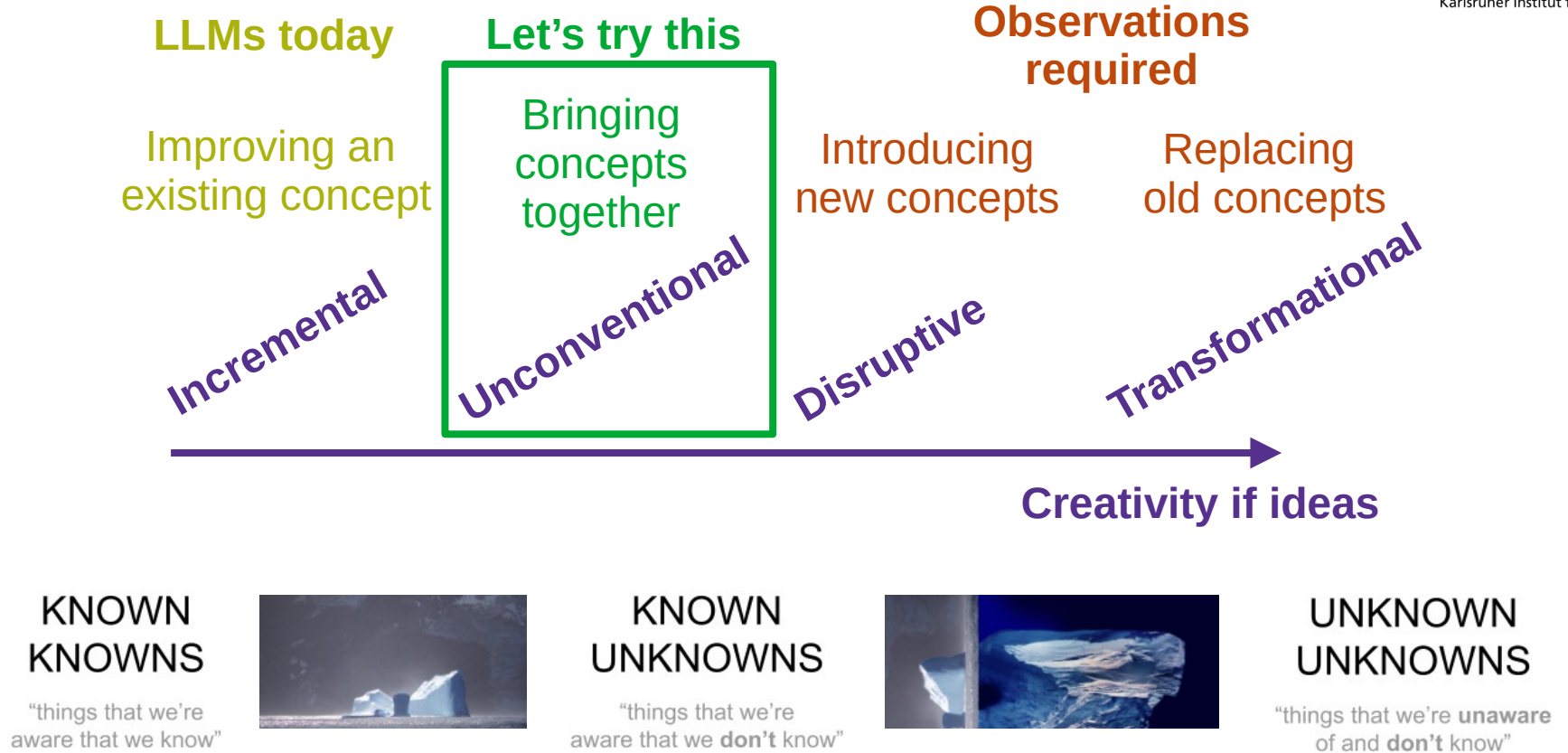


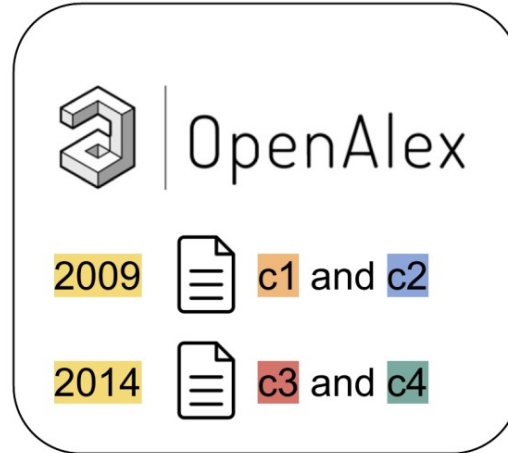
Image: Doug Belshaw, CC0

# From explanations to simpler models and new concepts

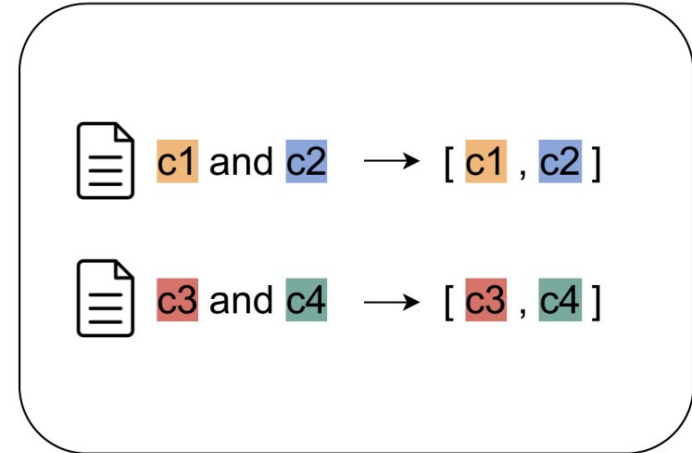
## Core materials science literature



**Thomas  
Marwitz**



**Dataset:**  
~221,000 papers



**Concept Extraction:**  
~137,000 concepts

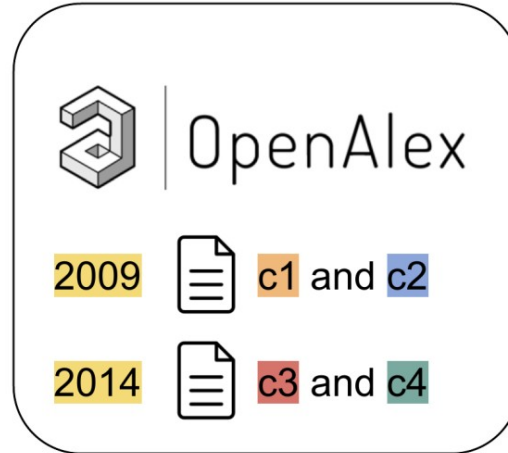
Marwitz *et al.*, **Nature Machine Intelligence** 2026  
arXiv:2506.16824

# From explanations to simpler models and new concepts

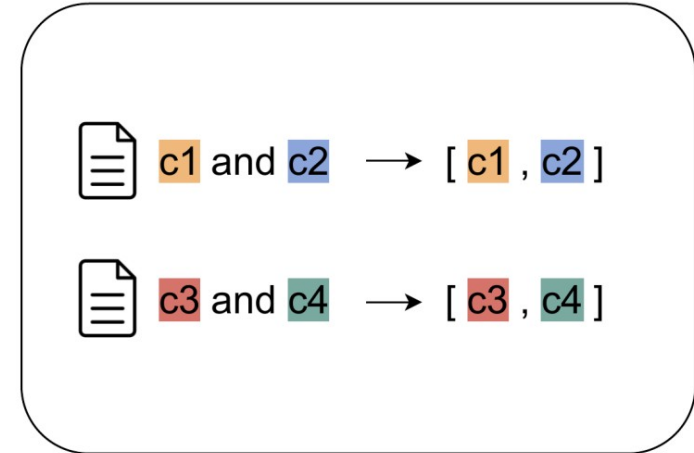
## Core materials science literature



**Thomas  
Marwitz**



**Dataset:**  
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### All of materials science and chemistry

- 11,000,000 papers
- 1,300,000 concepts (15+ occurrences)
- Coming soon...

Marwitz *et al.*, **Nature Machine Intelligence** 2026  
arXiv:2506.16824

# LLMs help with the extraction

Abstract excerpt	Extracted concept
"Strengthening mechanisms in short carbon fiber reinforced Nb/Nb <sub>5</sub> Si <sub>3</sub> composites"	carbon fiber reinforcement
"Removal of Metal Impurities from the"	metal impurity removal
"Resistance of Al <sub>2</sub> O <sub>3</sub> Coatings on Functional Structure"	al <sub>2</sub> o <sub>3</sub> coating
"Both fully and partially amorphous ribbons have been obtained"	fully amorphous ribbon, partially amorphous ribbon
"Successive ionic layer adsorption and reaction SILAR trend for"	successive ionic layer adsorption and reaction

Marwitz *et al.*, **Nature Machine Intelligence** 2026  
arXiv:2506.16824

# MAP of materials science

Explore all 137,000 concepts



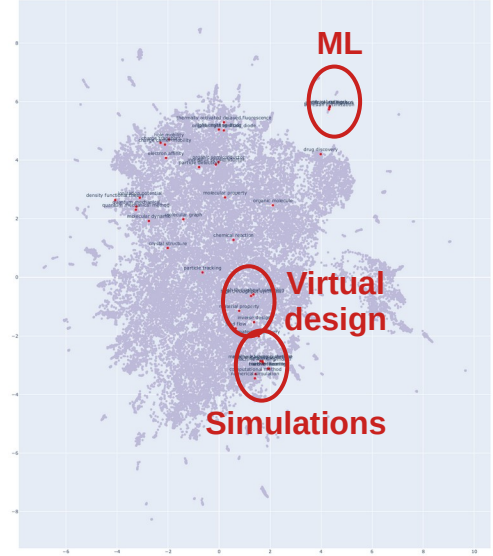
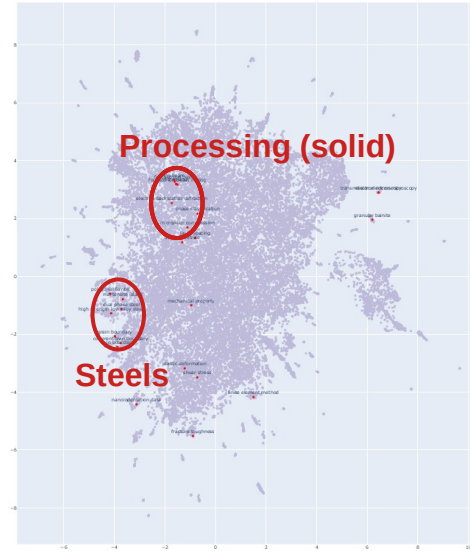
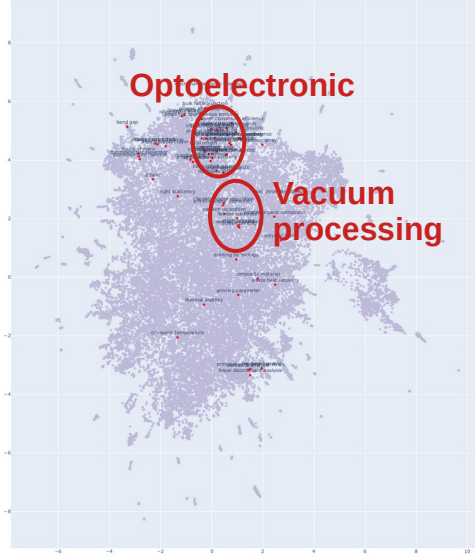
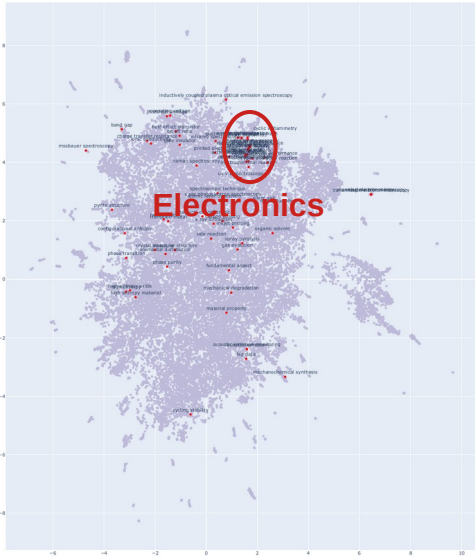
<http://inspire.aimat.science/>

Marwitz *et al.*, **Nature Machine Intelligence** 2026  
arXiv:2506.16824



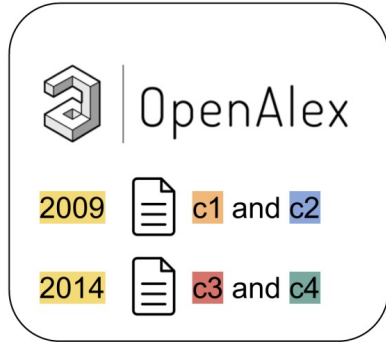
# MAP of materials science

Explore all 137,000 concepts

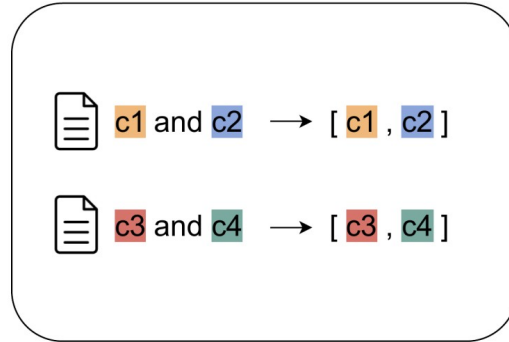


Marwitz *et al.*, **Nature Machine Intelligence** 2026  
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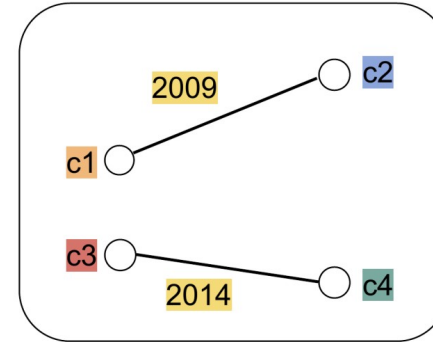
# From concepts to a concept graph



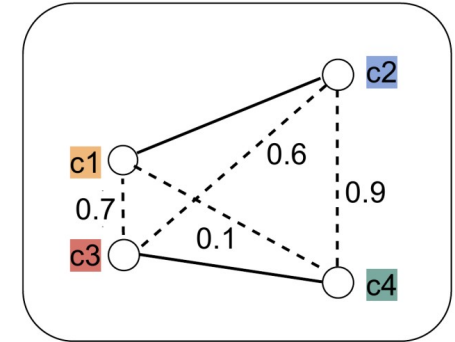
**Dataset:**  
~221,000 papers



**Concept Extraction:**  
~137,000 concepts



**Concept Graph:**  
~13,000,000 edges



**Link Prediction**



## Inspired by work of Mario Krenn

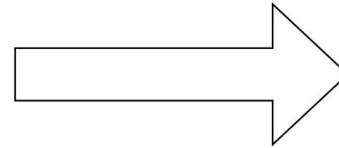
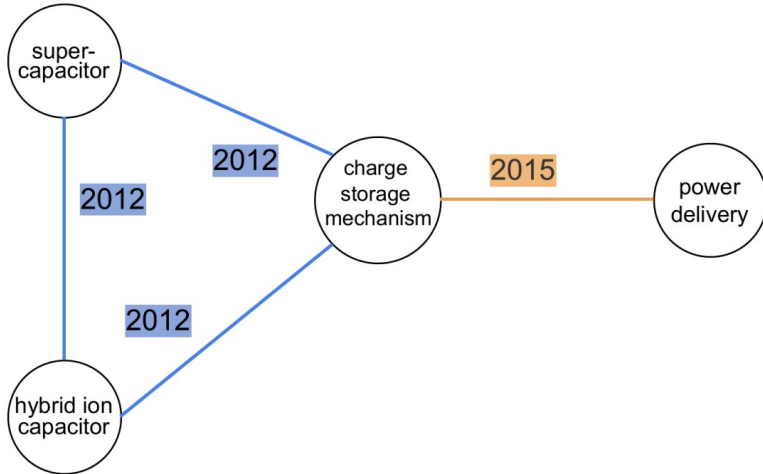
Nature Machine Intelligence 5, 1326–1335 (2023)

Marwitz *et al.*, Nature Machine Intelligence 2026

arXiv:2506.16824

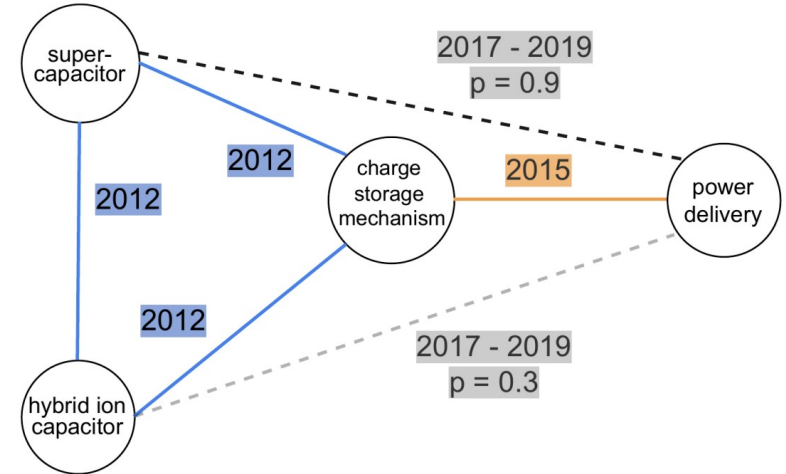
# New ideas are combinations of concepts

## Graph in 2016



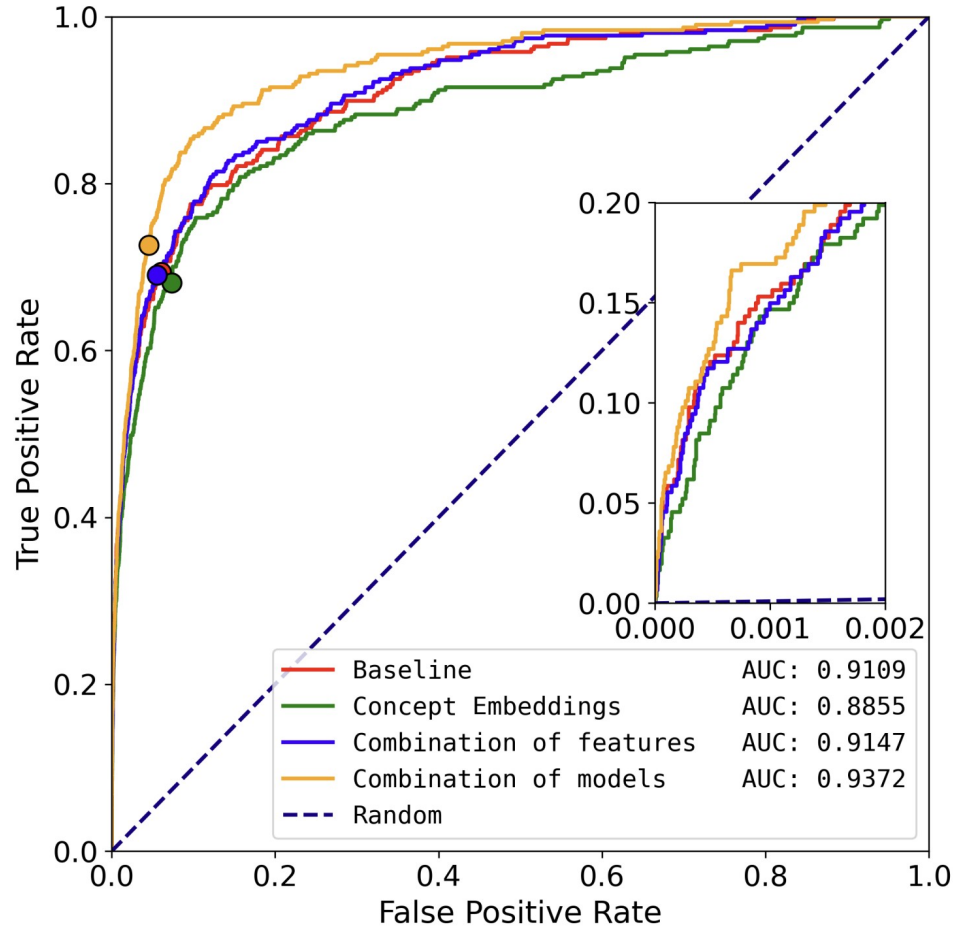
Link Prediction  
Model (NN)

## New links from 2017-2019

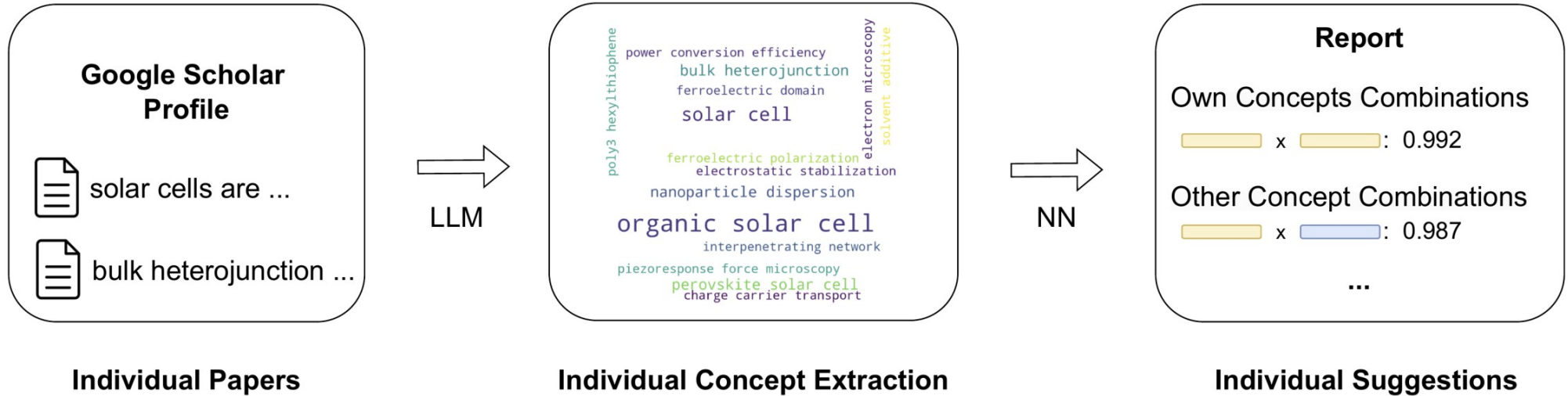


Marwitz *et al.*, **Nature Machine Intelligence** 2026  
arXiv:2506.16824

# New ideas are combinations of concepts



# Personalized recommendations



Marwitz *et al.*, **Nature Machine Intelligence** 2026  
arXiv:2506.16824

## Expert interviews

**A1:** known

**A2:** trivial

**B:** nonsense

**C:** interesting

Section	Category	Occurance	
		Number	Fraction
$S_{\text{own} \times \text{own}}$	A1	31	30.7%
	A2	21	20.8%
	B	25	24.8%
	C	24	23.7%
$S_{\text{own} \times \text{other}}$	A1	17	22.1%
	A2	8	10.4%
	B	35	45.4%
	C	17	22.1%

Marwitz *et al.*, **Nature Machine Intelligence** 2026

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# Personalized recommendations: Examples

"Conventional ceramic" + "Graphene oxide"



Ben Breitung

"Tensile strain" + "Molecular architecture"



Christoph  
Brabec

"Multiphase structure" + "Selective laser melting"



Horst Hahn

"In-plane polarization" + "Organic solar cell"



Alexander  
Colsmann

Christoph  
Kirchlechner



Try it yourself

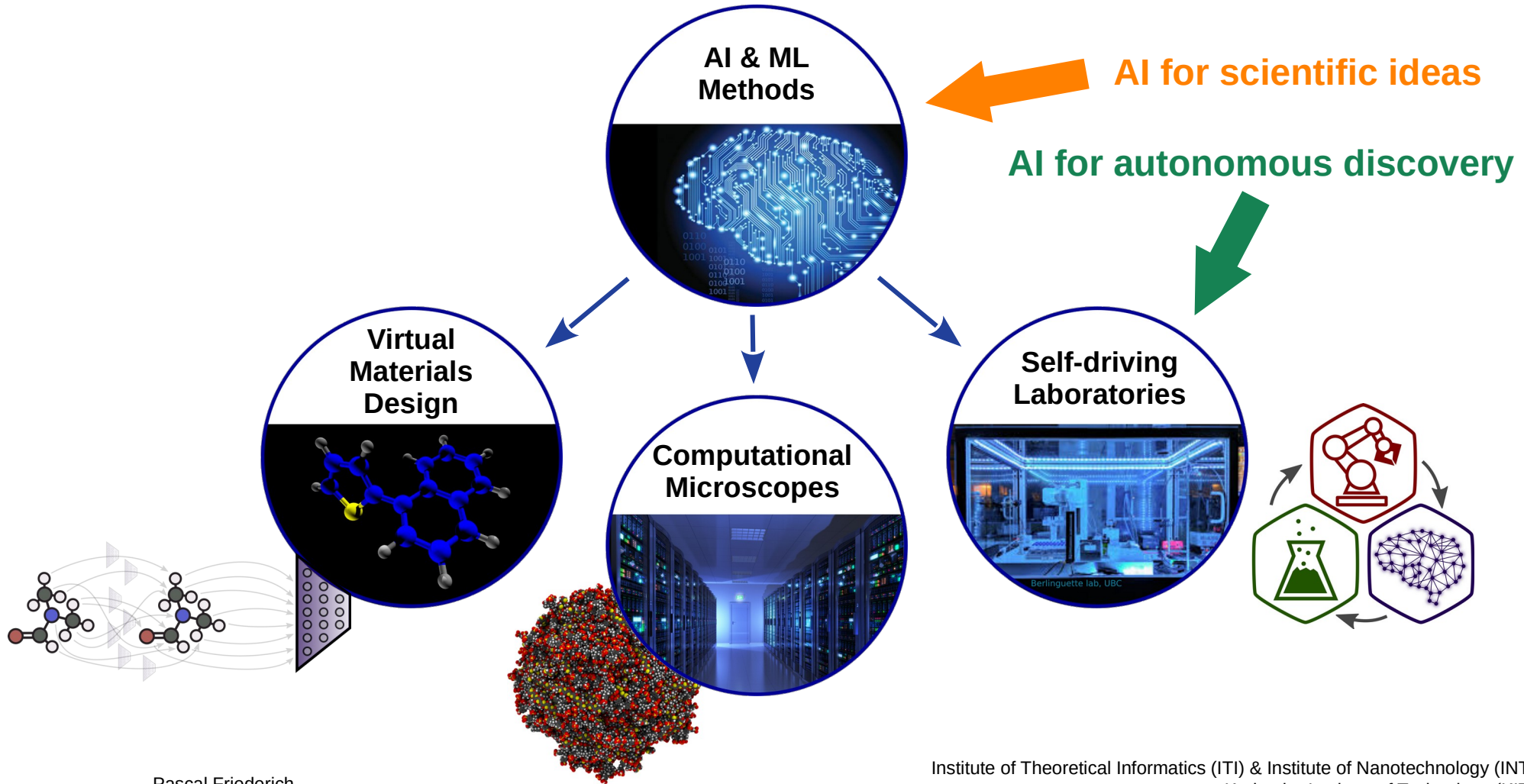


"Stress induced phase transformation" + "Hexagonal boron nitride"

Marwitz *et al.*, **Nature Machine Intelligence** 2026

arXiv:2506.16824

# Machine Learning for Materials Science and Chemistry



# Thank you for your attention!



Federal Ministry  
of Education  
and Research



HELMHOLTZ  
RESEARCH FOR GRAND CHALLENGES

