

AI for Materials Science: From Autonomous Materials Optimization to the Generation of Novel Ideas



Leibniz ScienceCampus
Digital Transformation
of Research

Pascal Friederich

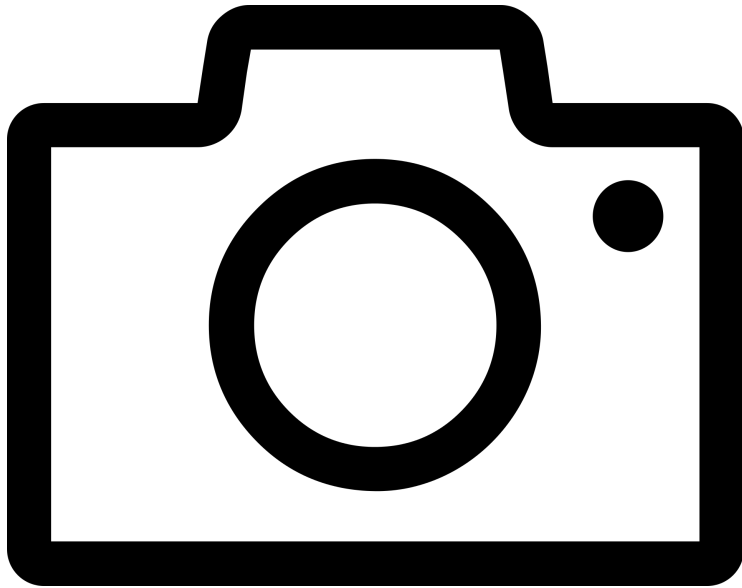
Institute of Nanotechnology, Karlsruhe Institute of Technology

Moderation: Linda Nierling (ITAS, KIT) & Katja Keller (IfSS, KIT)



Interdisciplinary Colloquium on Digitalisation of Research, 2nd of July 2026

Photos and recording



Pixabay, ste_phania



02.07.26 | 11:00-12:00

AI for Materials Science: From Autonomous Materials Optimization to the Generation of Novel Ideas



Pascal Friederich

Institute of Nanotechnology,
Karlsruhe Institute of
Technology

Outline

- AI and ML are transforming materials science and chemistry by accelerating materials and molecular discovery
- Pascal Friederich will present research that combines self-driving labs, automated data analysis, and autonomous experimental decision-making
- Beyond that, his team uses large language models and concept graphs to predict emerging research directions in materials science



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

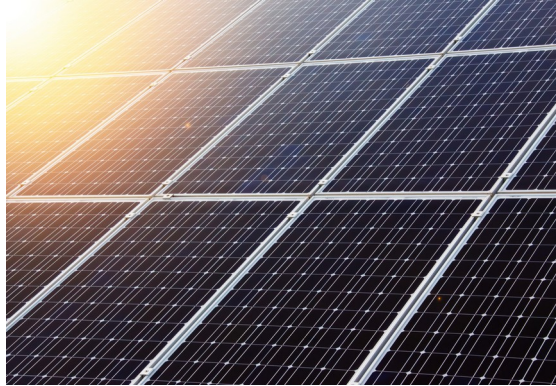
Email: pascal.friederich@kit.edu

Web: aimat.science

2 July 2026

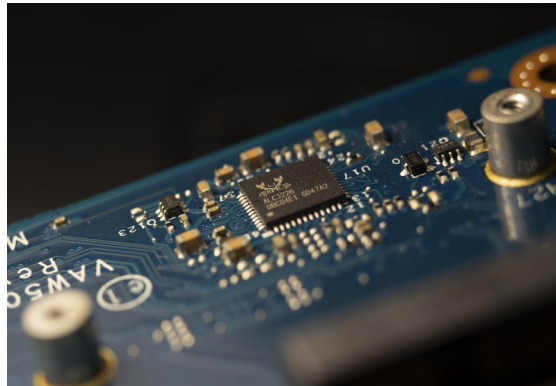
Materials are the driver for innovation

Renewable energy
Photovoltaics
Batteries



By PublicDomainPictures via Pixabay

Electronics
Chips
Semiconductors



By Henryphoto via Pixabay



By padrinan via Pixabay

Medicine
Antibiotics
Vaccines



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



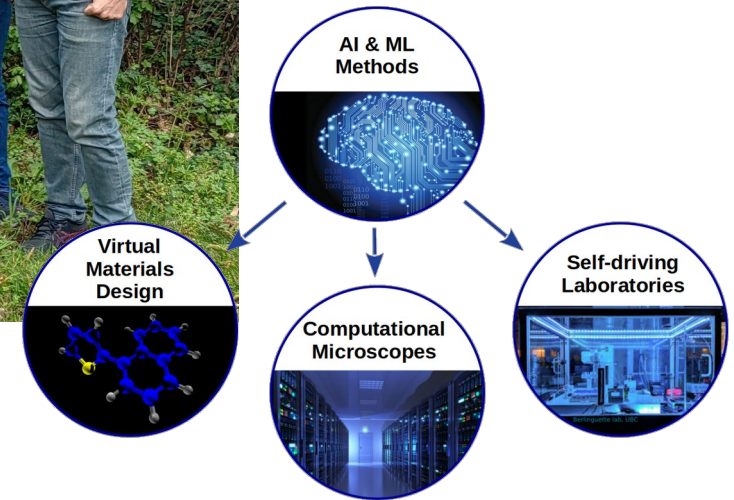
<https://sdgs.un.org/goals>

Research group AI for Materials Science (AiMat)

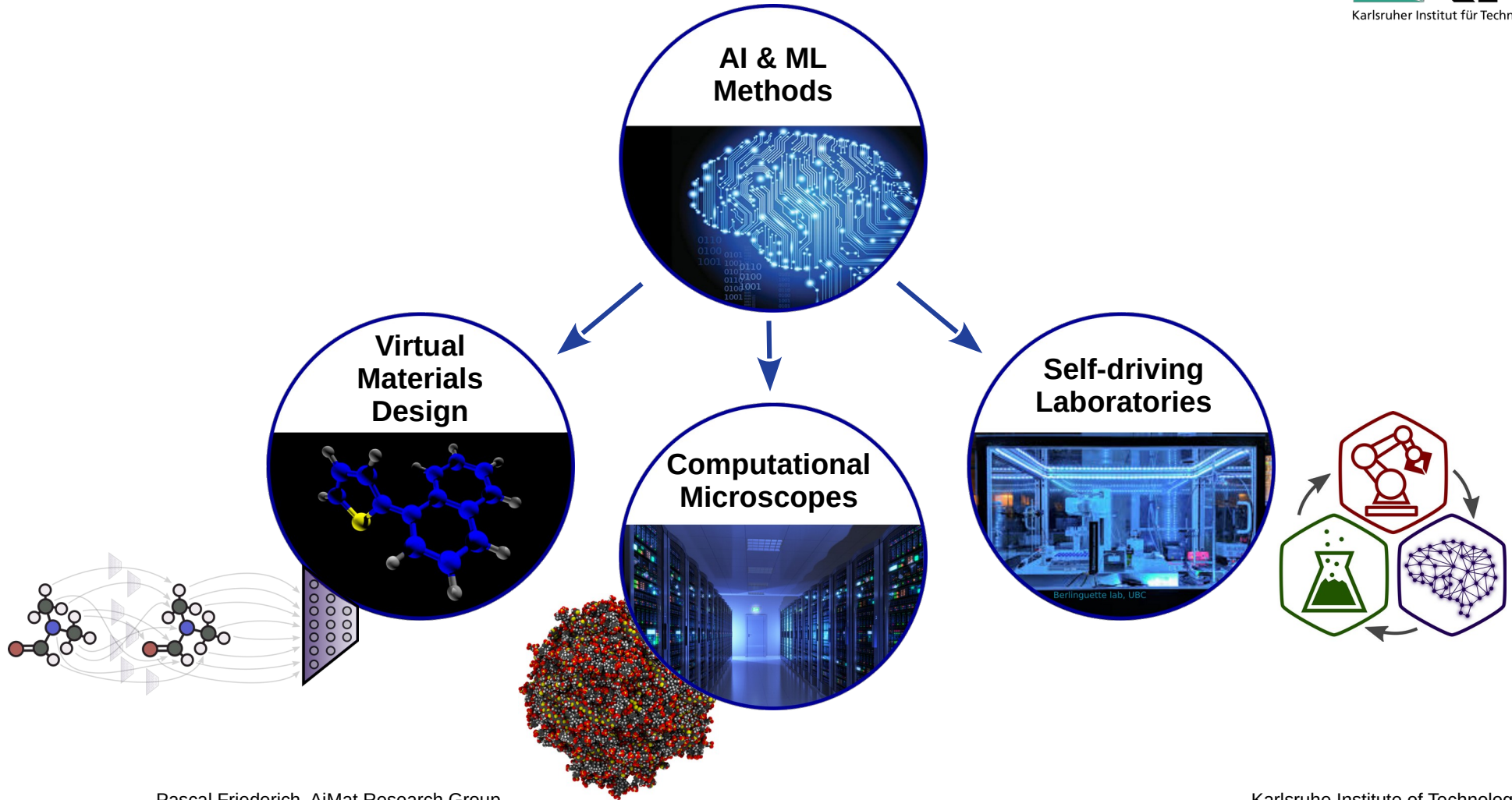


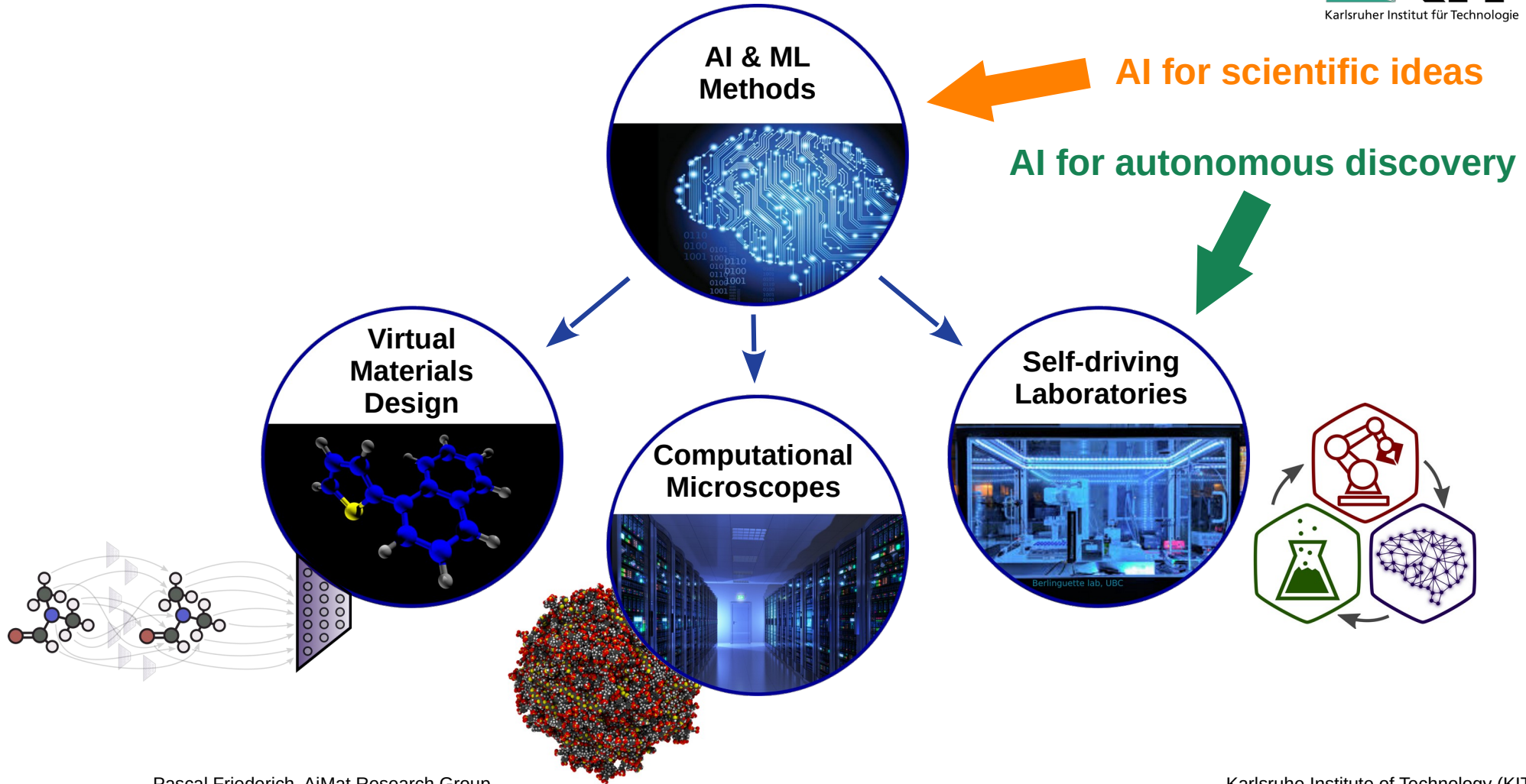
Bridge between

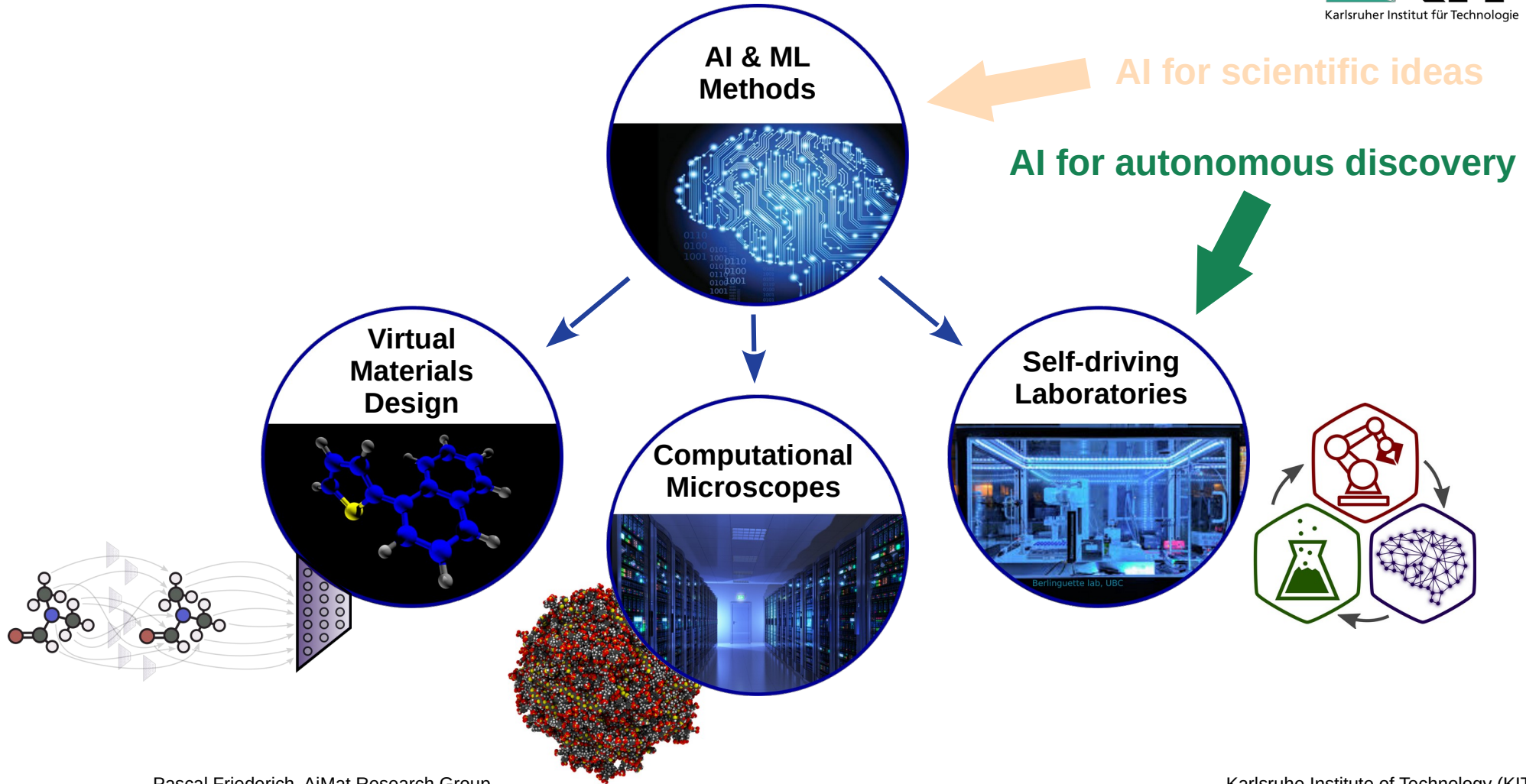
- **Methods development in computer science**
- **Applications in materials science and chemistry**



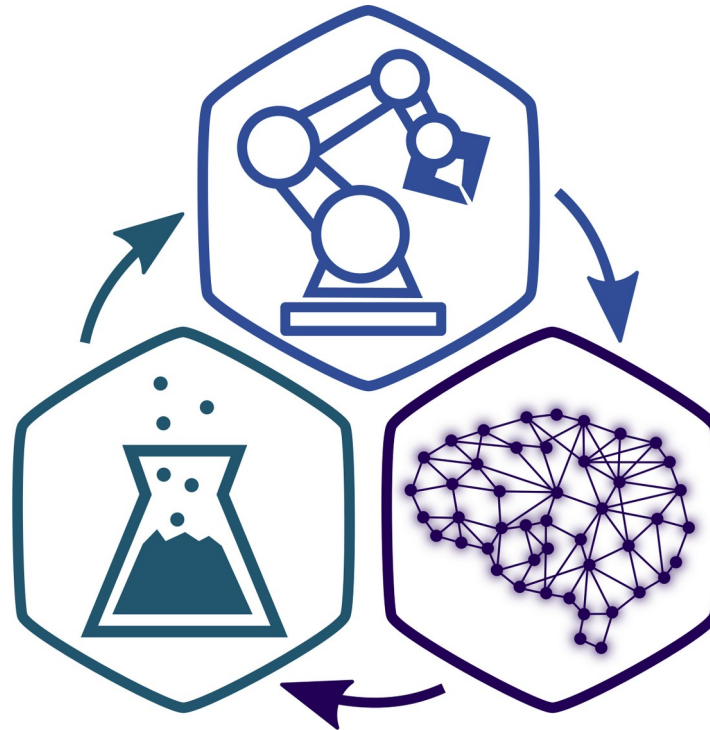
Machine Learning for Materials Science and Chemistry







Idea



Closing the loop

AI for Autonomous Experiments

Ceramics for additive manufacturing

Collaboration with

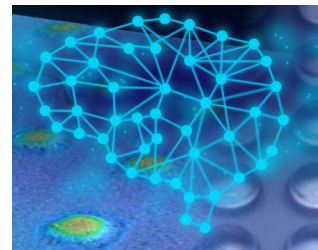
Karlsruher Institut für Technologie
Schubert *et al.*,
Open Ceramics 2024.



Responsive polymers

Collaboration with

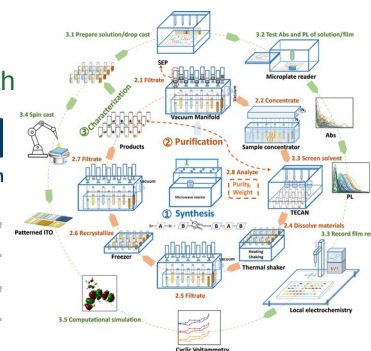
Karlsruher Institut für Technologie
Seifermann *et al.*,
Small Methods 2023.



Photovoltaics materials

Collaboration with

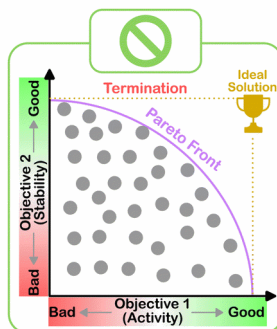
Wu *et al.*,
JACS 2023.
Wu *et al.*,
Science 2024.



Catalyst development

Collaboration with

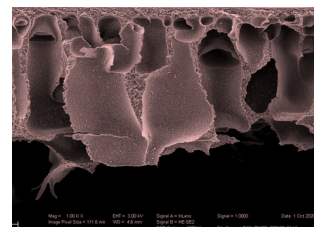
Jenewein *et al.*,
J. Mat. Chem. A 2023.



Filtration membrane design

Collaboration with

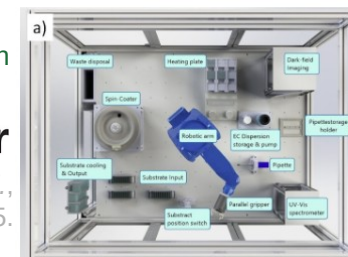
Glass *et al.*,
ACS Appl. Mater. Interfaces 2024.



Electrochromic films

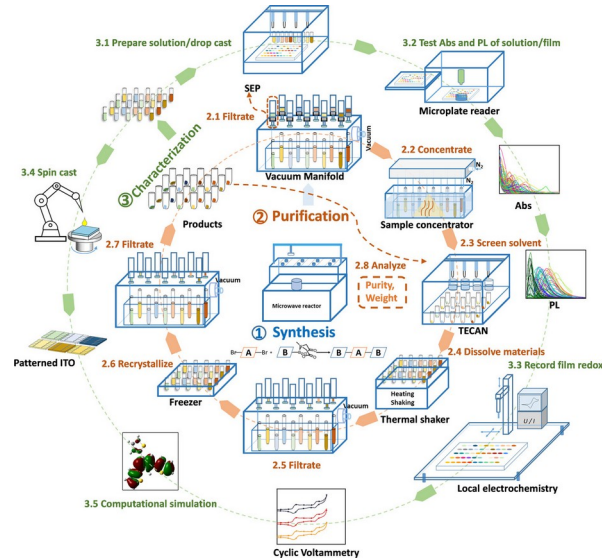
Collaboration with

Dahms *et al.*,
In preparation 2025.



Design of solar cell materials

From synthesis ...



...to devices!



[10.1021/acs.accounts.4c00095](https://doi.org/10.1021/acs.accounts.4c00095)

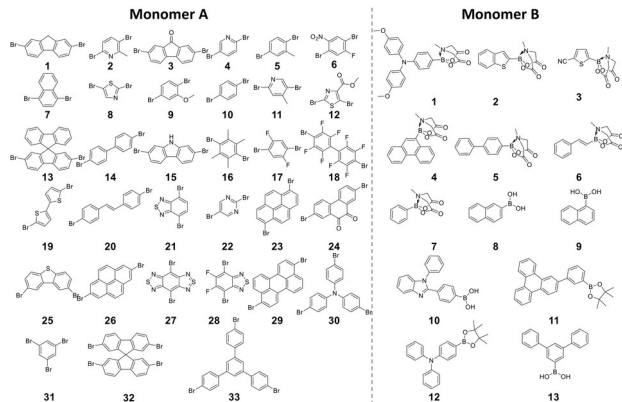
FAU
Friedrich-Alexander-Universität
Erlangen-Nürnberg



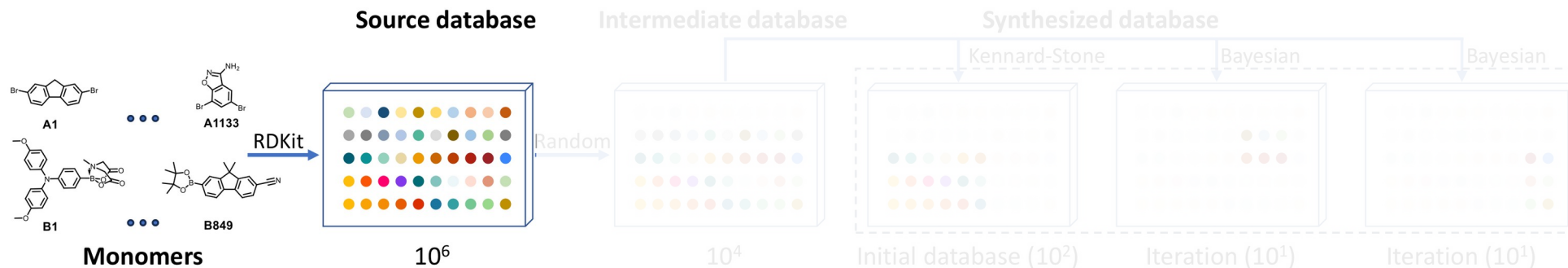
**Christoph
Brabec**

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

Synthesis in a space of 1,000,000 molecules

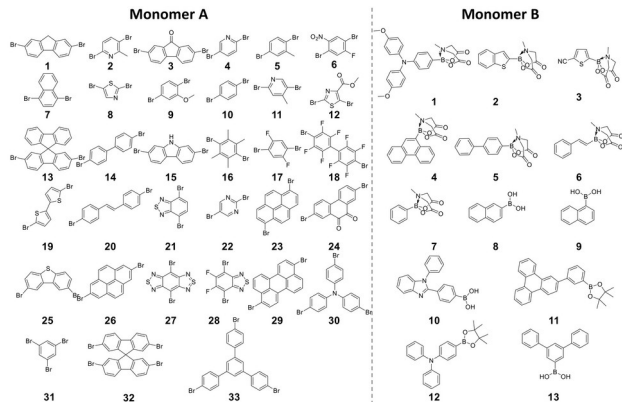


- Hole transport materials for **perovskite solar cells**
 - Automated synthesis of A-B-A molecules
 - Library of ~1000 A and ~1000 B fragments
- **Chemical space of 1,000,000 molecules**



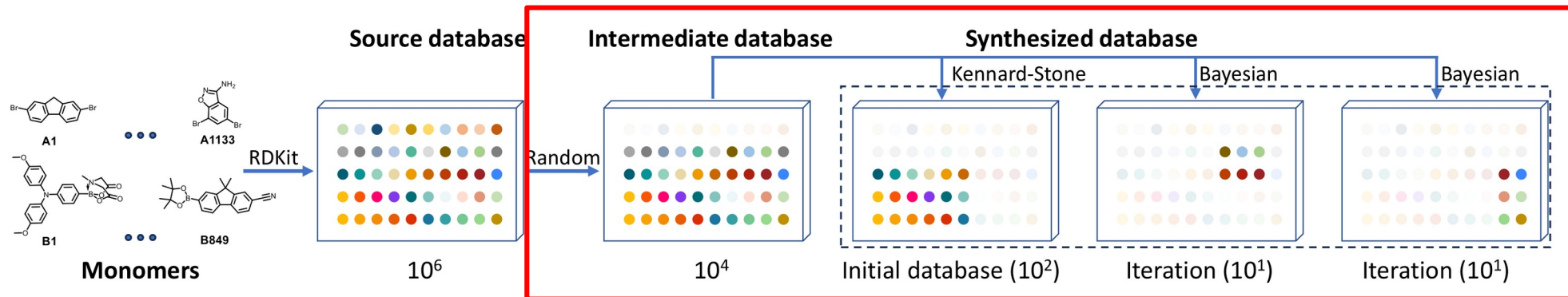
Wu, Friederich, Brabec *et al.*, JACS, **2023**.
Wu, Friederich, Brabec *et al.*, Science, **2024**.

Synthesis in a space of 1,000,000 molecules



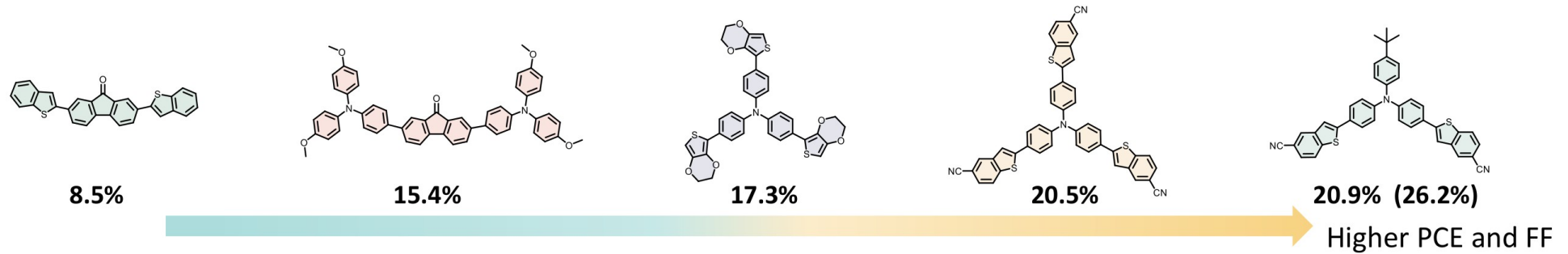
- Hole transport materials for **perovskite solar cells**
- Automated synthesis of A-B-A molecules
- Library of ~1000 A and ~1000 B fragments
→ **Chemical space of 1,000,000 molecules**

Autonomous exploration



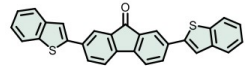
Wu, Friederich, Brabec *et al.*, JACS, **2023**.
Wu, Friederich, Brabec *et al.*, Science, **2024**.

Optimization of device performance through HTL design

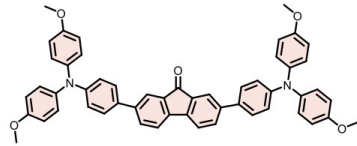


Wu, Friederich, Brabec *et al.*, JACS, **2023**.
Wu, Friederich, Brabec *et al.*, Science, **2024**.

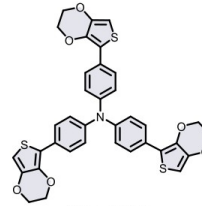
Optimization of device performance through HTL design



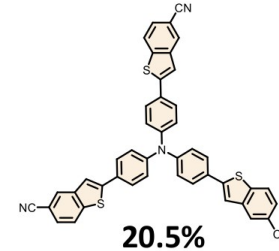
8.5%



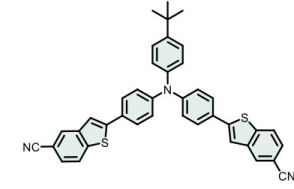
15.4%



17.3%

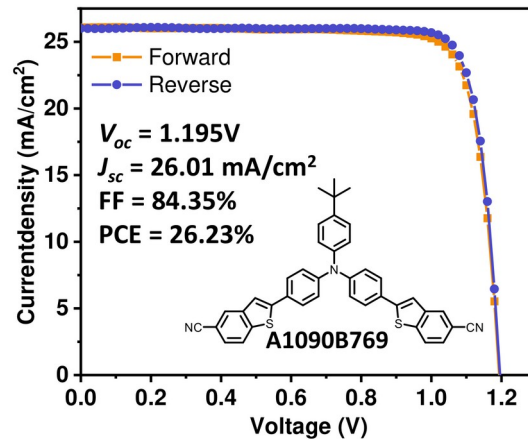


20.5%



20.9% (26.2%)

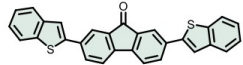
Higher PCE and FF



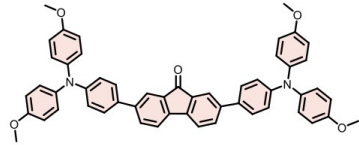
Performance in optimized device: 26.2%

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

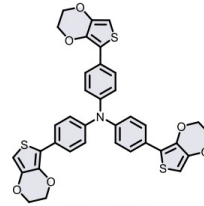
Optimization of device performance through HTL design



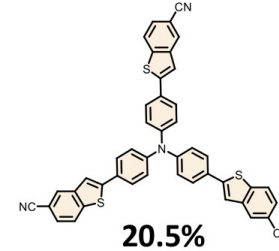
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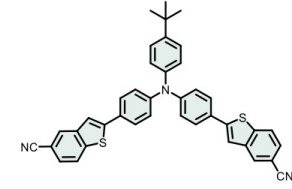
15.4%



17.3%

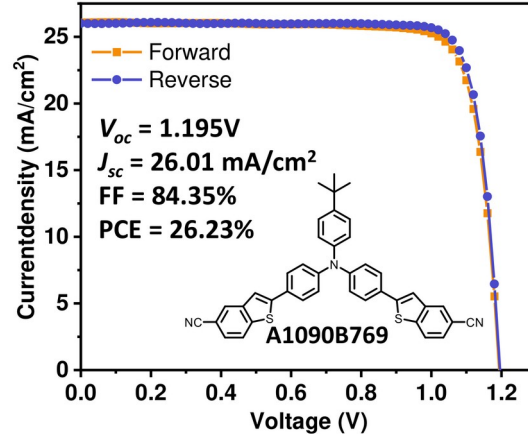


20.5%

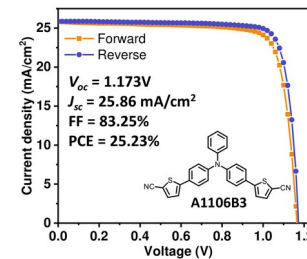
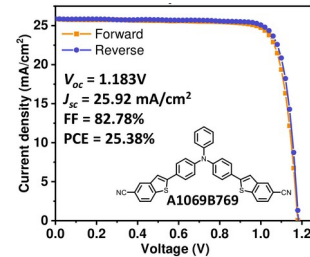


20.9% (26.2%)

Higher PCE and FF



Multiple candidates with >25% efficiency!



...

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

HELMA HELMHOLTZ Acceleration Alliance

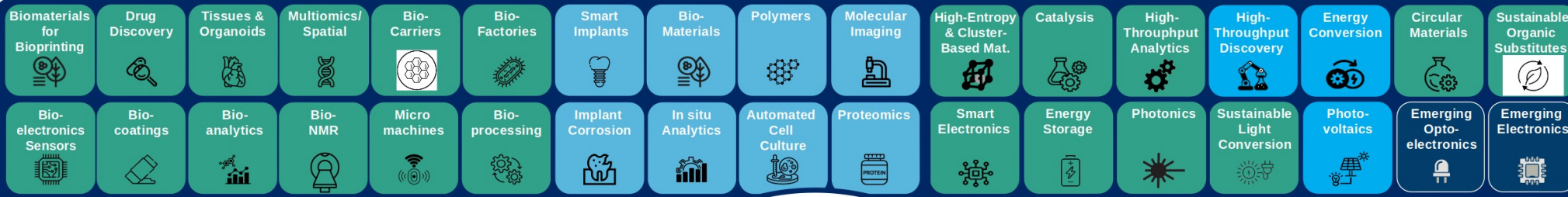
**Think Bigger and Faster:
The Helmholtz Acceleration Alliance**



HELMHOLTZ Information

Decentralized Self Driving Lab Network

Health Technologies (HealthTech)



Helmholtz Biomedical Engineering

Partners from **Helmholtz Health**

Accelerated & Autonomous Material Discovery (A2MD)



Partners from **Helmholtz Energy**

Tech Lab



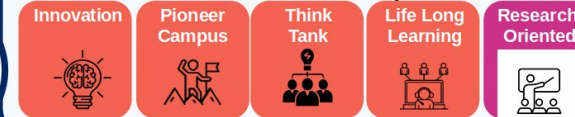
AI Lab



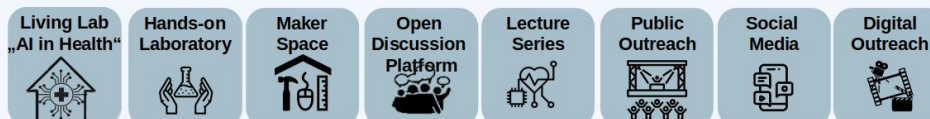
HELMHOLTZ QUANTUM



Pioneer Campus



Outreach



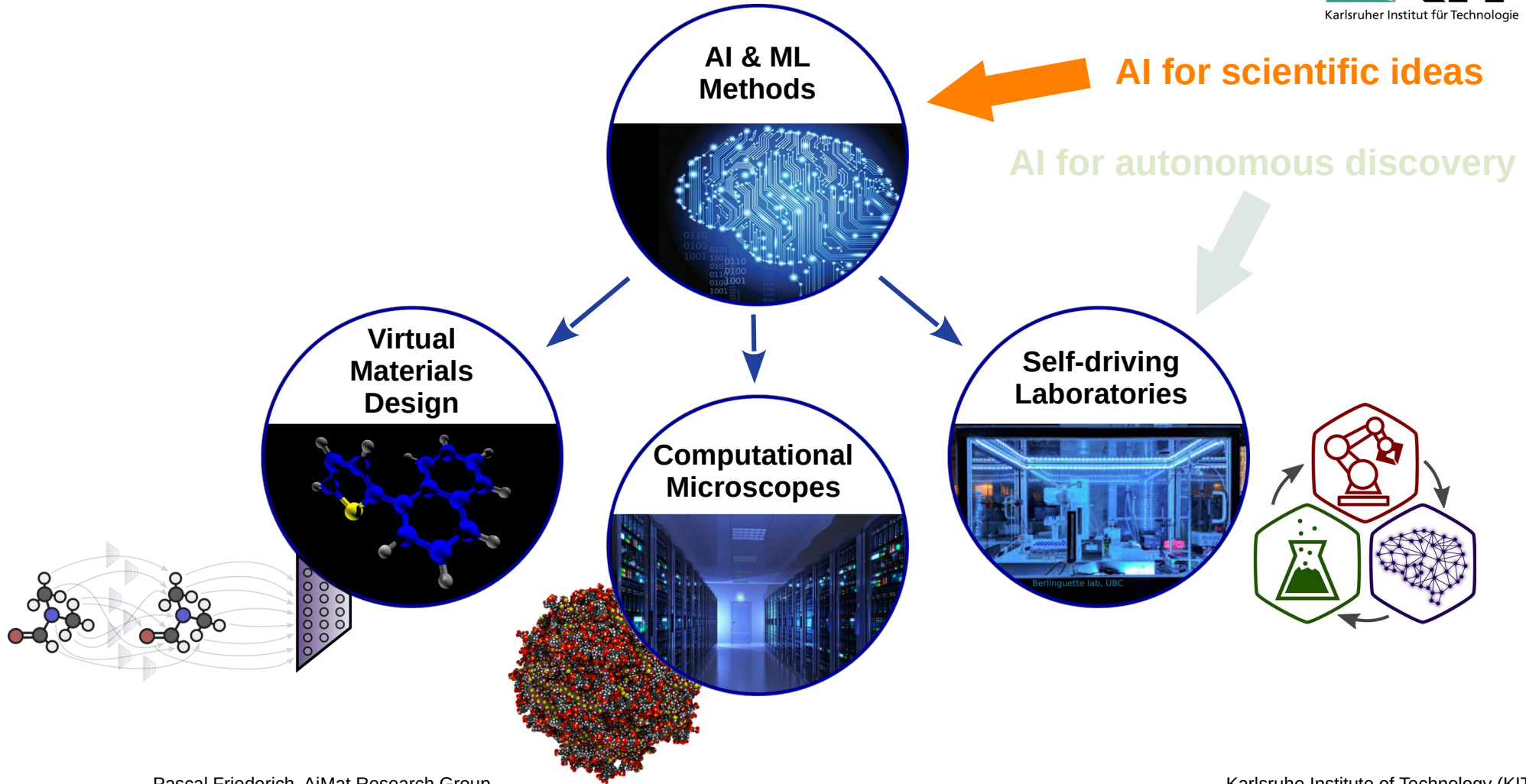




Image: Doug Belshaw, CC0, <https://blog.dougbelshaw.com/solving-complexity>
Wikimedia Commons, <https://de.wikipedia.org/wiki/Datei:Iceberg.jpg>

Scientific progress

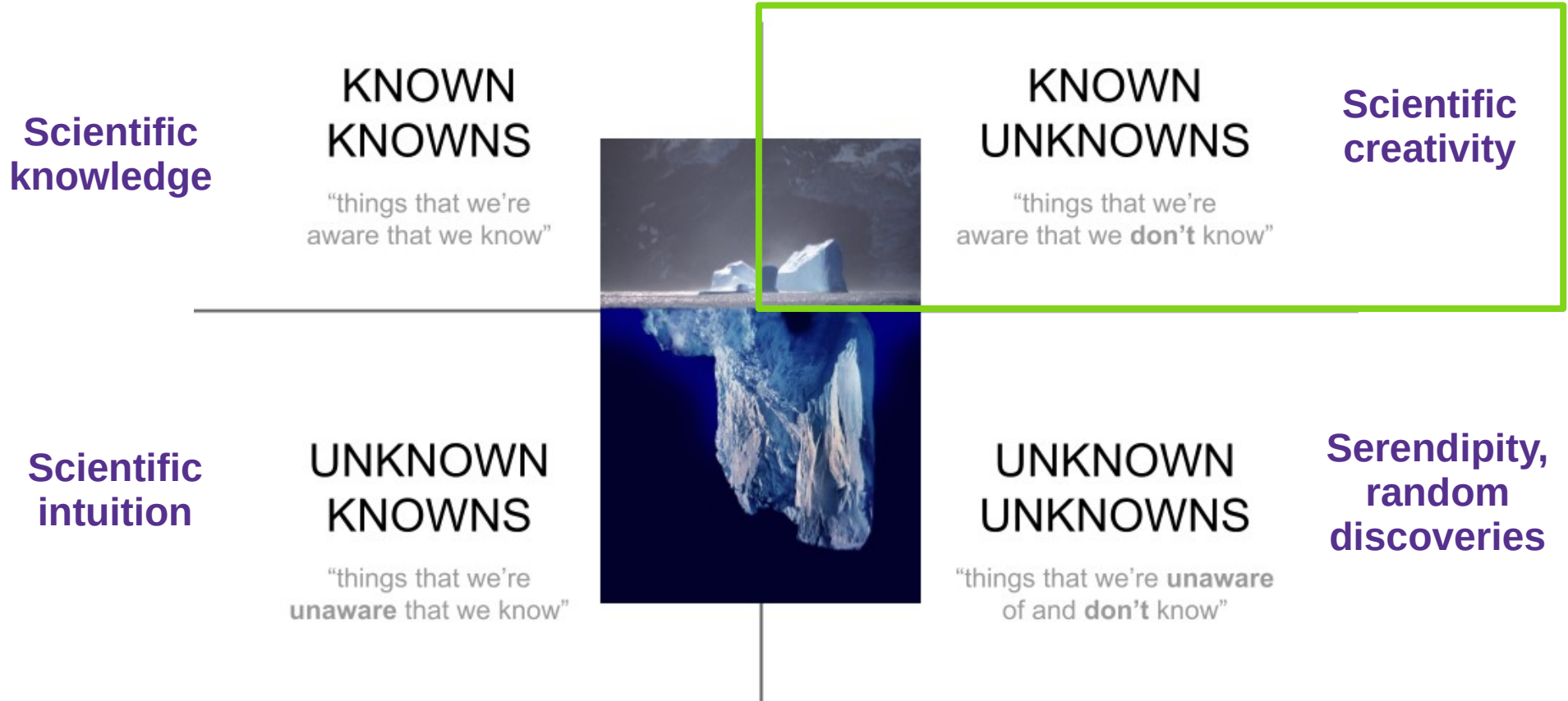


Image: Doug Belshaw, CC0

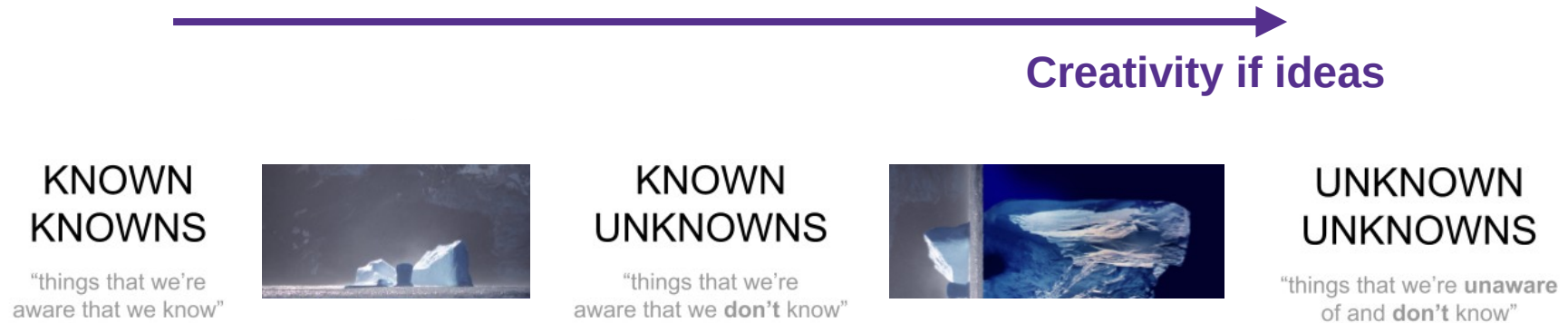


Image: Doug Belshaw, CC0

Improving an
existing concept

Incremental

Creativity if ideas

**KNOWN
KNOWNS**

“things that we’re
aware that we know”



**KNOWN
UNKNOWNs**

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



**UNKNOWN
UNKNOWNs**

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

Image: Doug Belshaw, CC0

Creation of scientific ideas

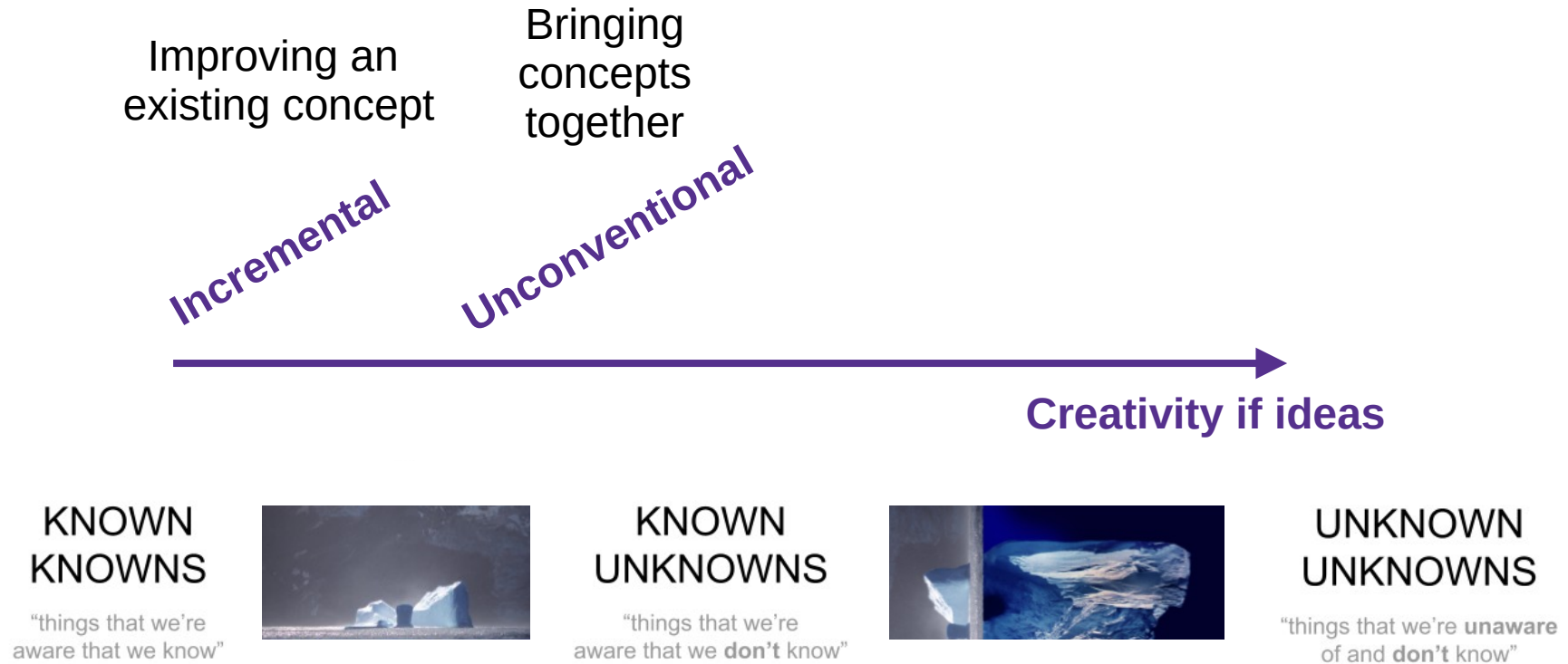


Image: Doug Belshaw, CC0

Creation of scientific ideas

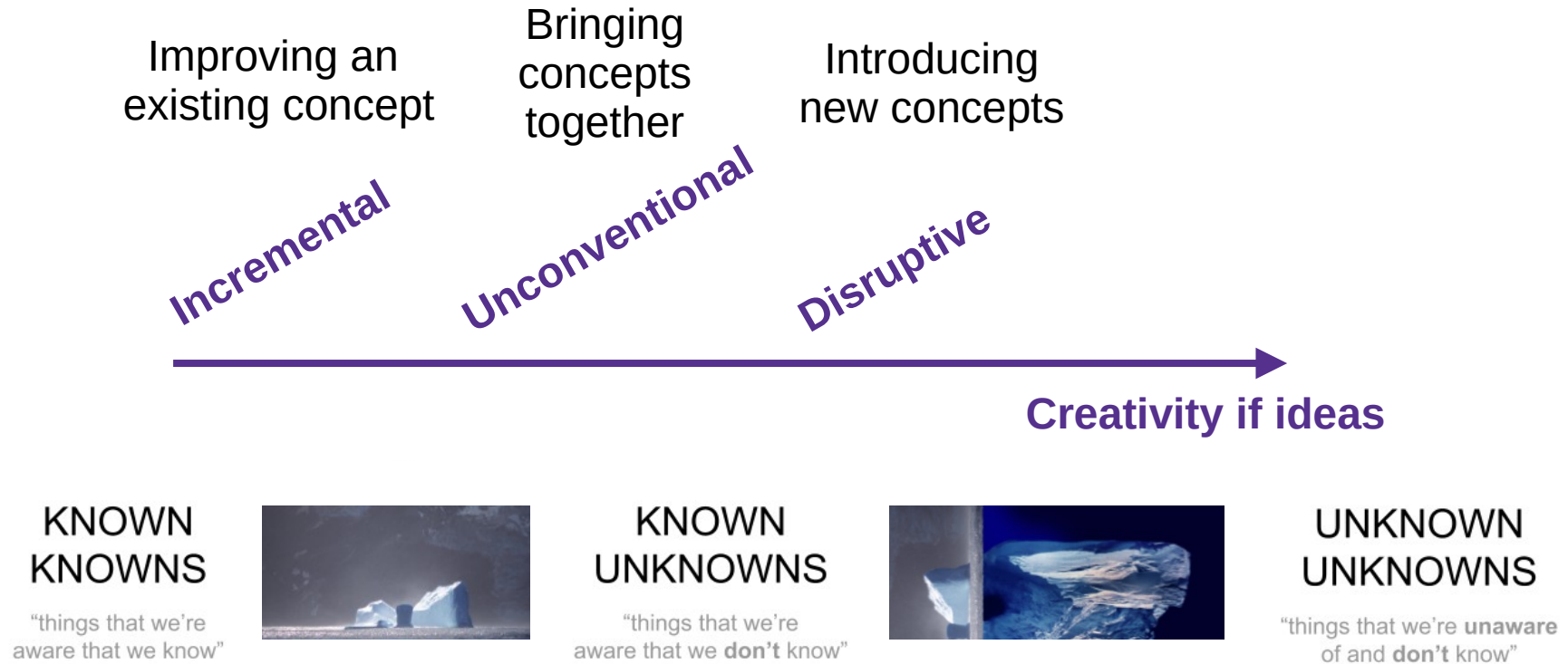


Image: Doug Belshaw, CC0

Creation of scientific ideas

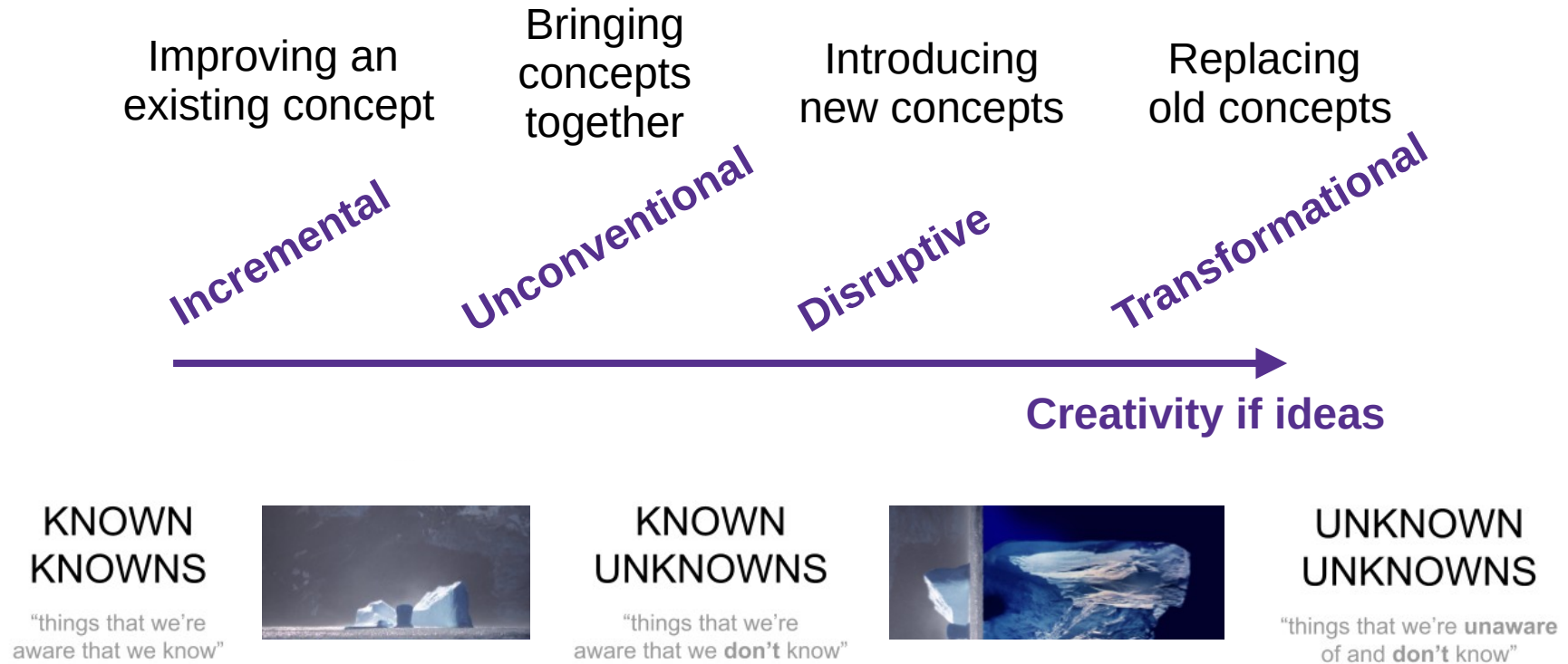


Image: Doug Belshaw, CC0

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

KNOWN
KNOWNS

“things that we’re
aware that we know”



KNOWN
UNKNOWN

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



UNKNOWN
UNKNOWN

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

Image: Doug Belshaw, CC0

Creation of scientific ideas

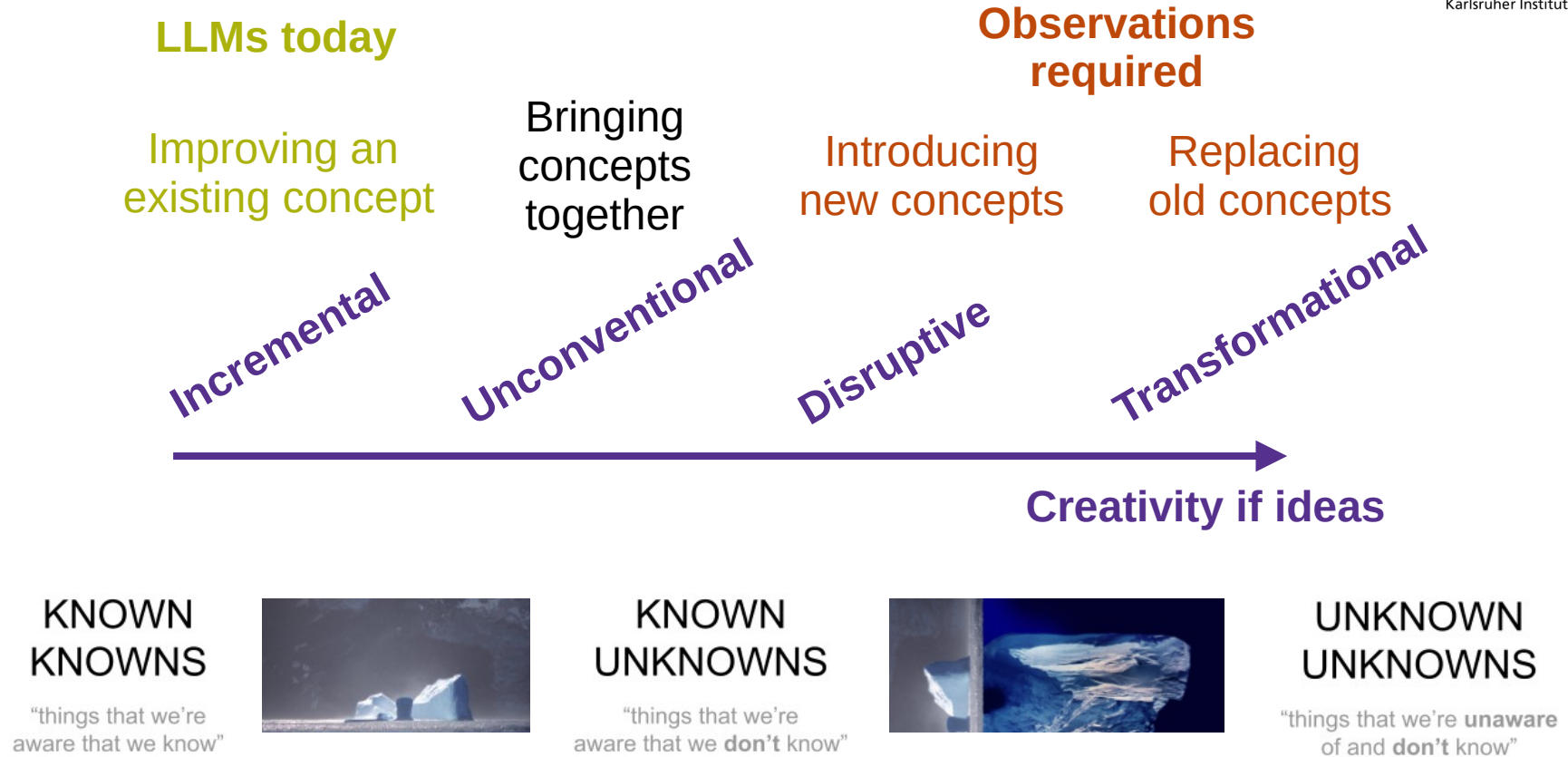


Image: Doug Belshaw, CC0

Creation of scientific ideas

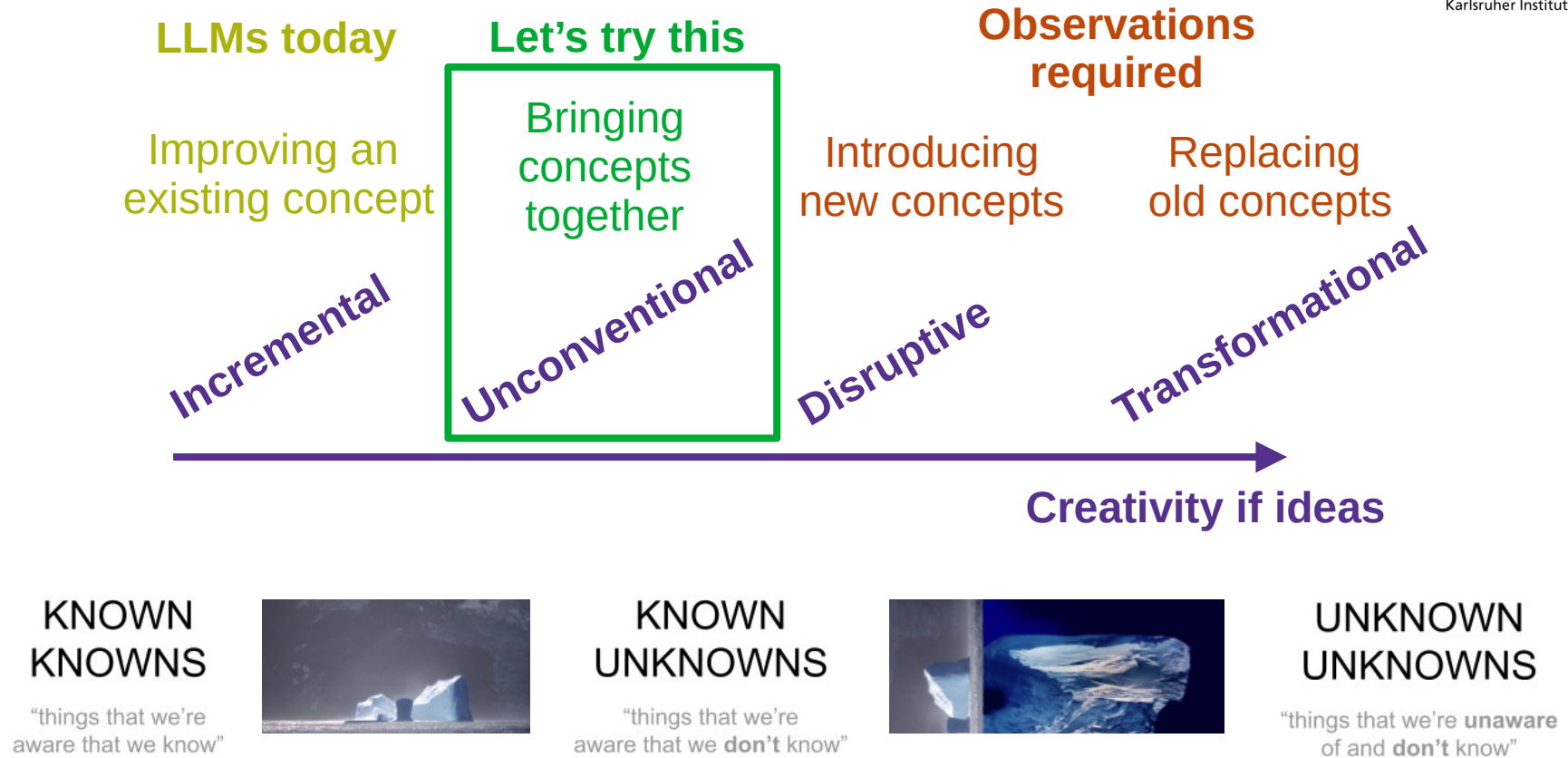


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From explanations to simpler models and new concepts

Core materials science literature



**Thomas
Marwitz**

 | OpenAlex

2009  c1 and c2

2014  c3 and c4

Dataset:
~221,000 papers

 c1 and c2 $\rightarrow$ [c1 , c2]

 c3 and c4 $\rightarrow$ [c3 , c4]

Concept Extraction:
~137,000 concepts

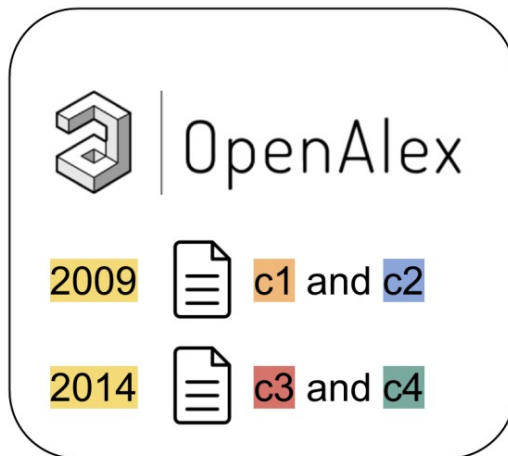
Marwitz *et al.*, **Nature Machine Intelligence** 2026
arXiv:2506.16824

From explanations to simpler models and new concepts

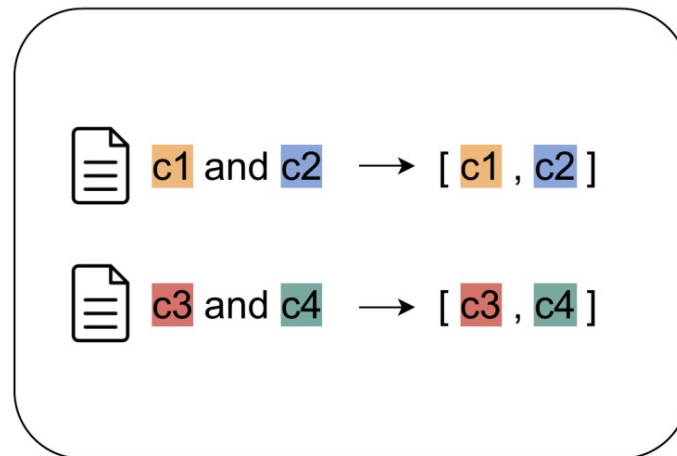
Core materials science literature



**Thomas
Marwitz**



Dataset:
~221,000 papers



Concept Extraction:
~137,000 concepts

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

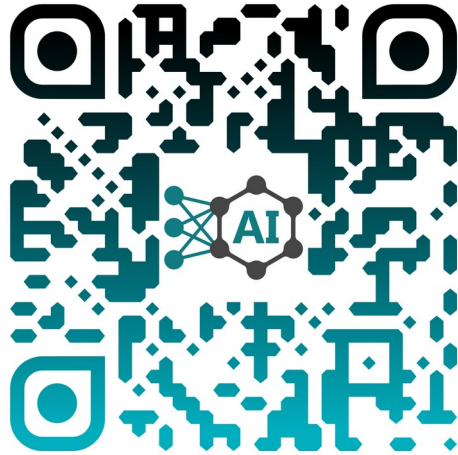
LLMs help with the extraction

Abstract excerpt	Extracted concept
"Strengthening mechanisms in short carbon fiber reinforced Nb/Nb ₅ Si ₃ composites"	carbon fiber reinforcement
"Removal of Metal Impurities from the"	metal impurity removal
"Resistance of Al ₂ O ₃ Coatings on Functional Structure"	al ₂ o ₃ 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



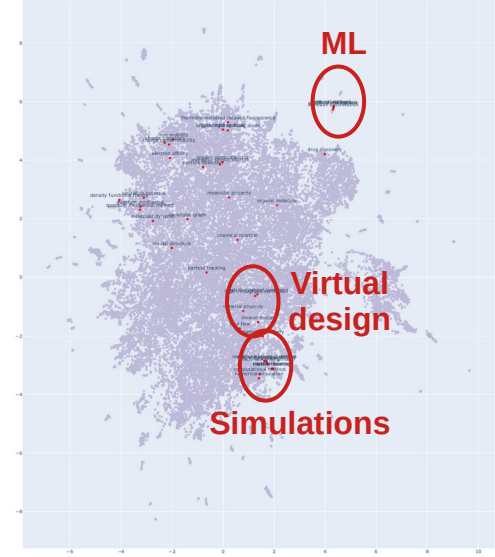
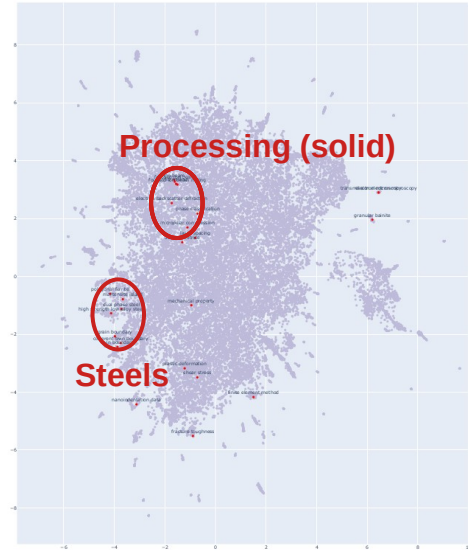
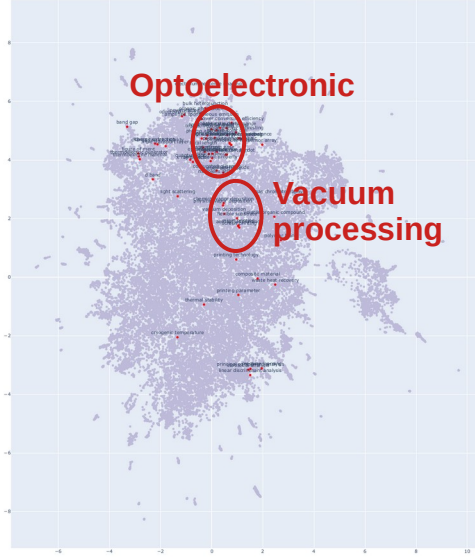
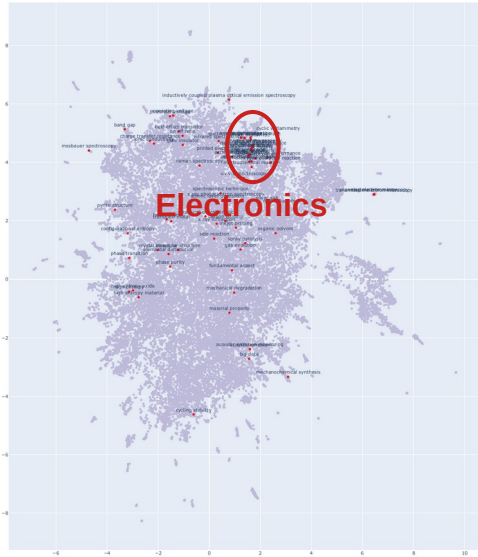
<http://inspire.aimat.science/>

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



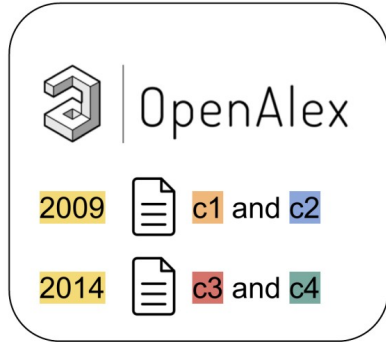
MAP of materials science

Explore all 137,000 concepts

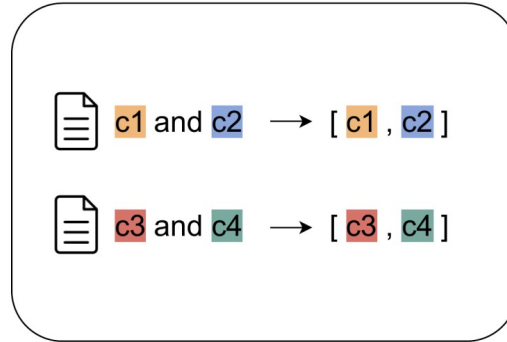


Marwitz *et al.*, **Nature Machine Intelligence** 2026
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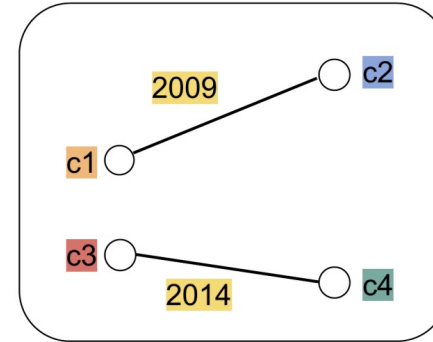
From concepts to a concept graph



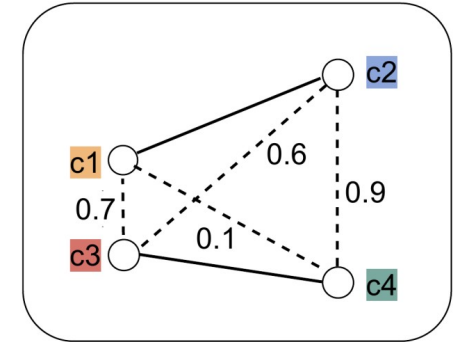
Dataset:
~221,000 papers



Concept Extraction:
~137,000 concepts



Concept Graph:
~13,000,000 edges



Link Prediction

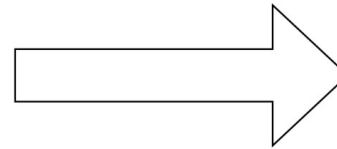
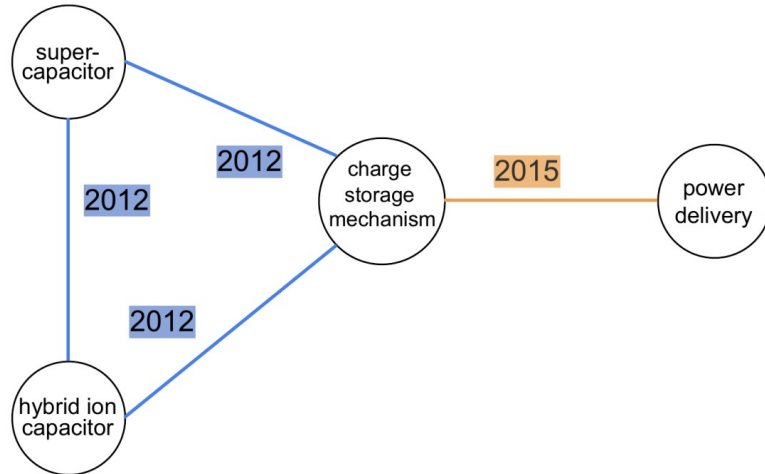


Inspired by work of Mario Krenn
Nature Machine Intelligence 5, 1326–1335 (2023)

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

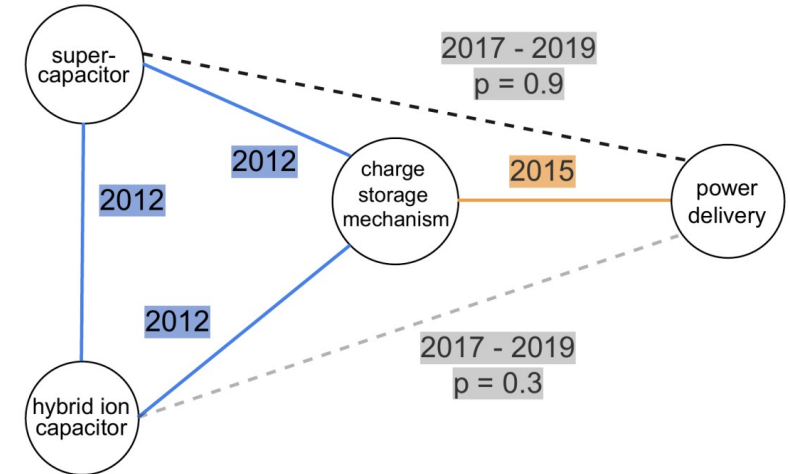
New ideas are combinations of concepts

Graph in 2016



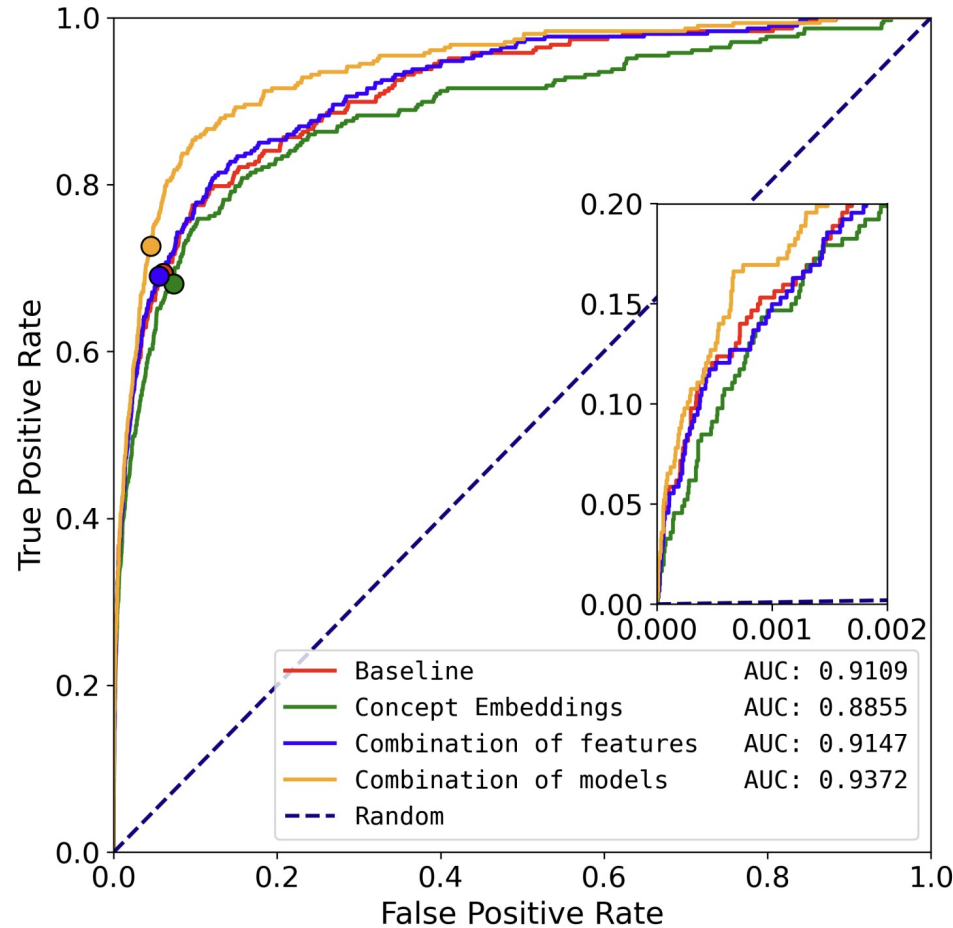
Link Prediction
Model (NN)

New links from 2017-2019



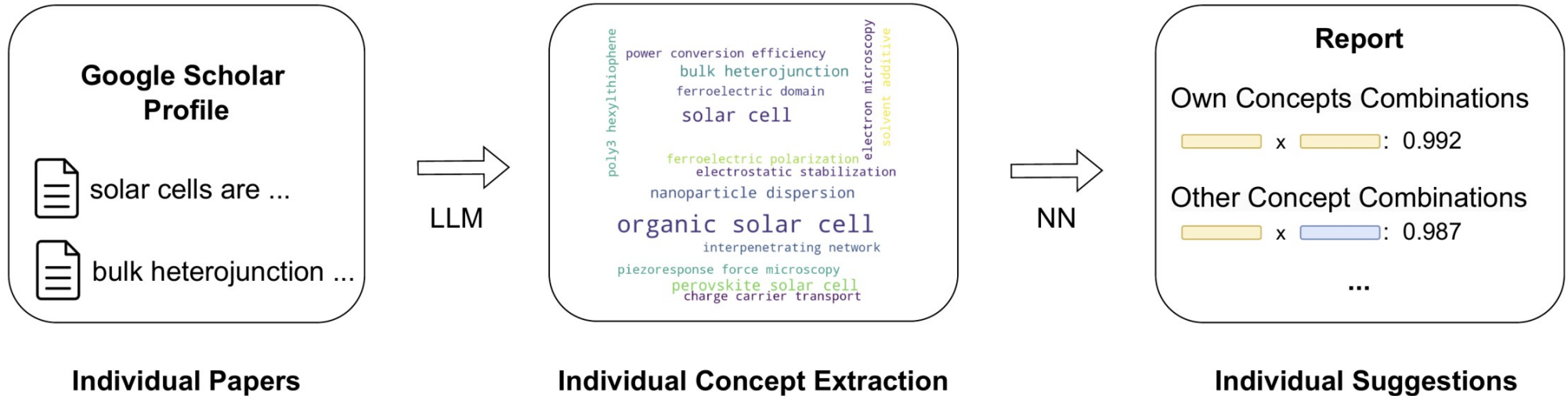
Marwitz *et al.*, **Nature Machine Intelligence** 2026
arXiv:2506.16824

New ideas are combinations of concepts



Nature Machine Intelligence 2026
arXiv:2506.16824

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
arXiv:2506.16824

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



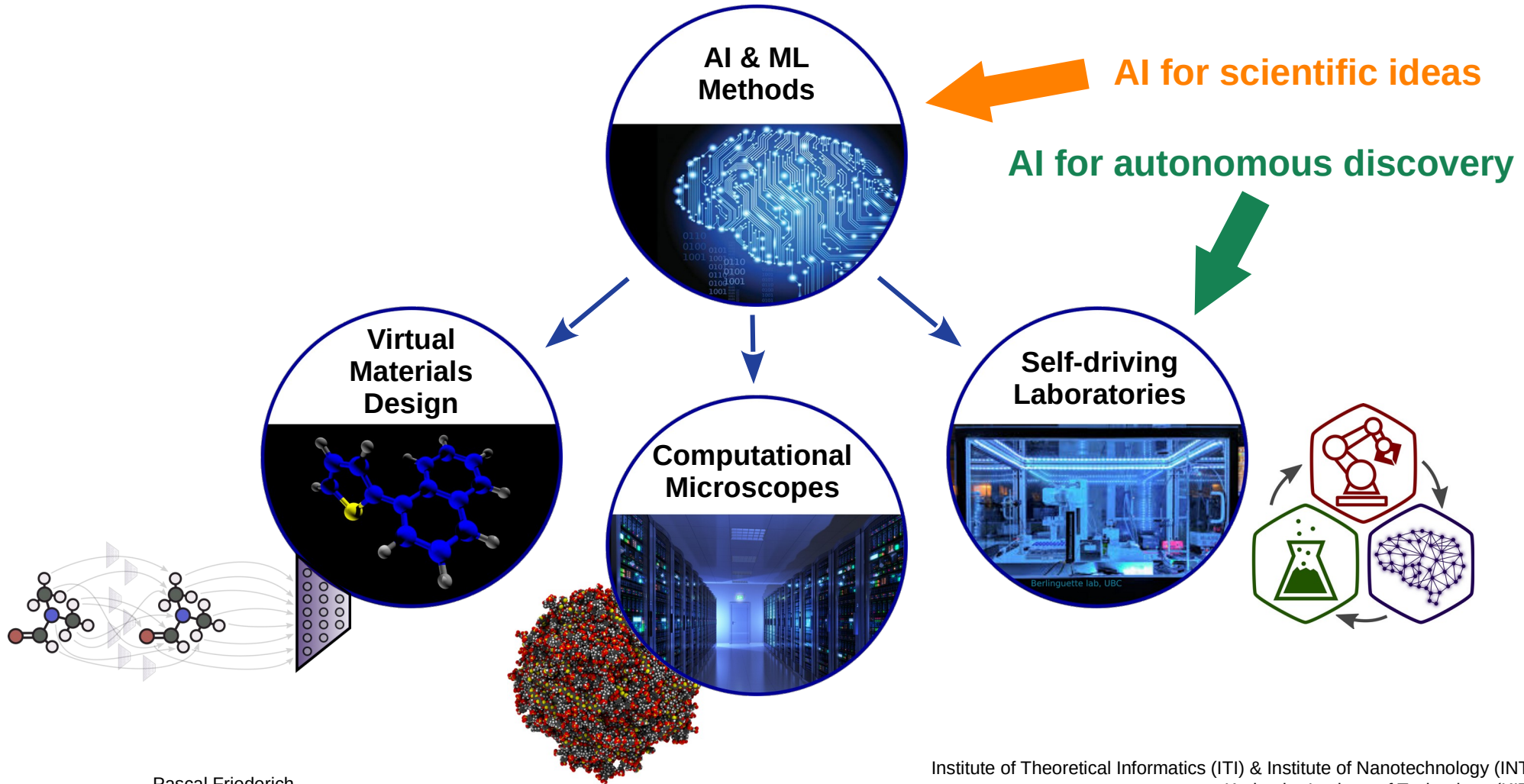
Try it yourself



"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!



Discussion Session

Next Colloquium

is with **Signe Mezinska** from the Institute of
Clinical and Preventive Medicine, University of
Latvia

6th of August 2026
save the date

Save the date!

DiTraRe Interdisciplinary Symposium 2: 6-7 April 2027



Save the date for our second Interdisciplinary Symposium on Digitalisation of Research, which will take place in Karlsruhe at KIT from 6 to 7 April 2027!

Thank you for joining!

Stay connected

- DiTraRe
 - Website: www.ditrare.de/en
 - Email: ditrare@fiz-karlsruhe.de
 - LinkedIn: www.linkedin.com/company/ditrare
 - Mastodon: social.kit.edu/@DiTraRe
 - YouTube: www.youtube.com/@DiTraRe
 - Zenodo: zenodo.org/communities/ditrare
- Discussion forum: www.ditrare.de/en/forum
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