eosc

Scientific keynote: FAIR, what else?

Claudia Draxl

Professor for solid-state theory at the Physics Department of the Humboldt-Universität zu Berlin and Director of FAIRMAT

Federal Ministry of Education and Research
eosc Focus
Funded by the European Union
In cooperation with
nfdi
ZBW Leibniz-Informationszentrum Wirtschaft Leibniz Information Centre for Economics

NOMAD

FAIR, what else?

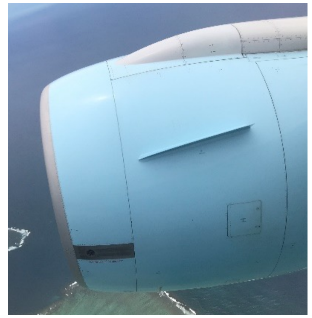
Claudia Draxl

Findable & AI Ready

Materials, materials, ...

Materials are decisive for every aspect of our society

Lighting



Transportation

Communication

Tools

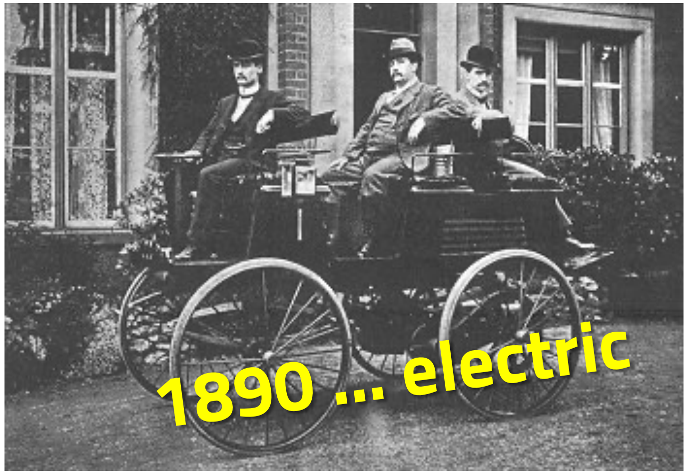
Entertainment

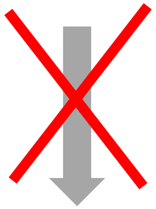
Computing

Light harvesting

Health

Our environment ...





Have you thought about recycling?

How green is our research?

What do we find in publications?

A table?

A figure?

A structure?

A few numbers?

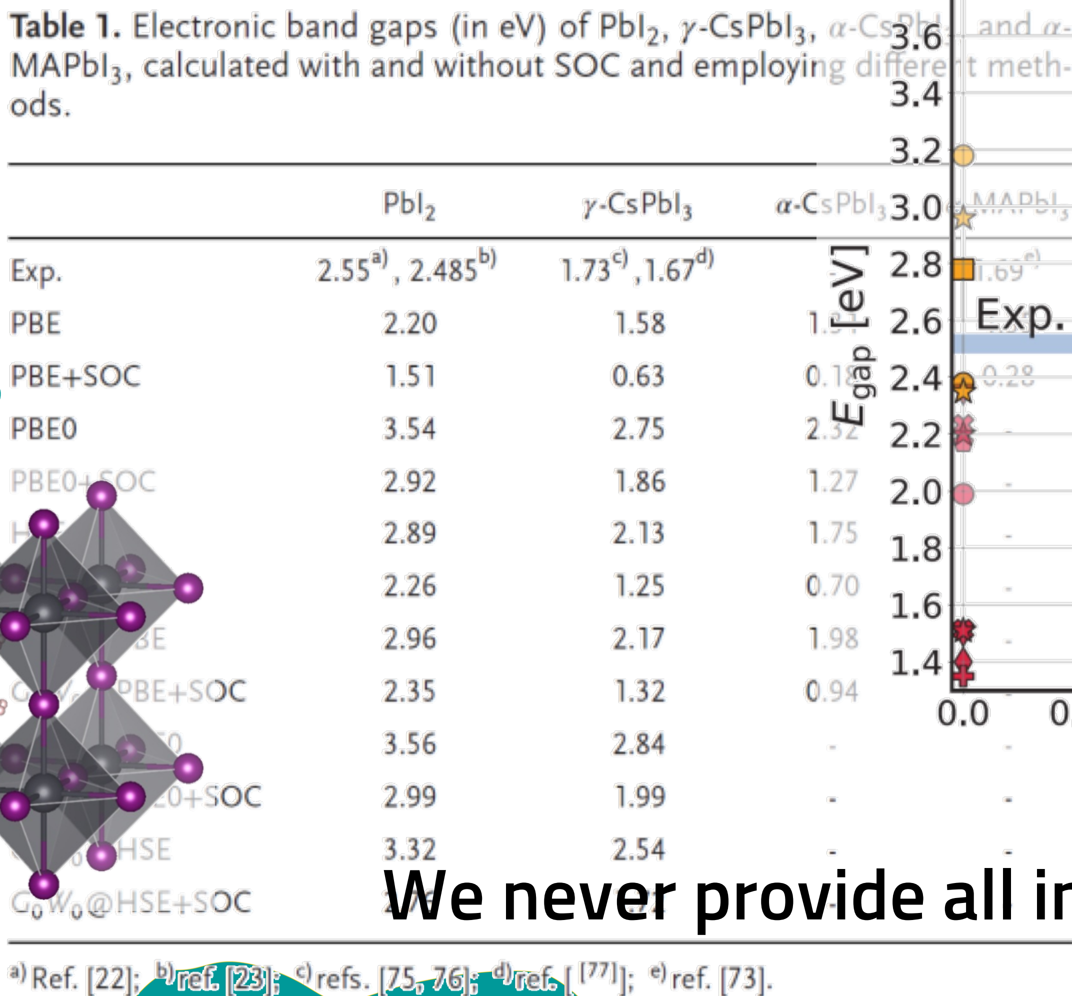
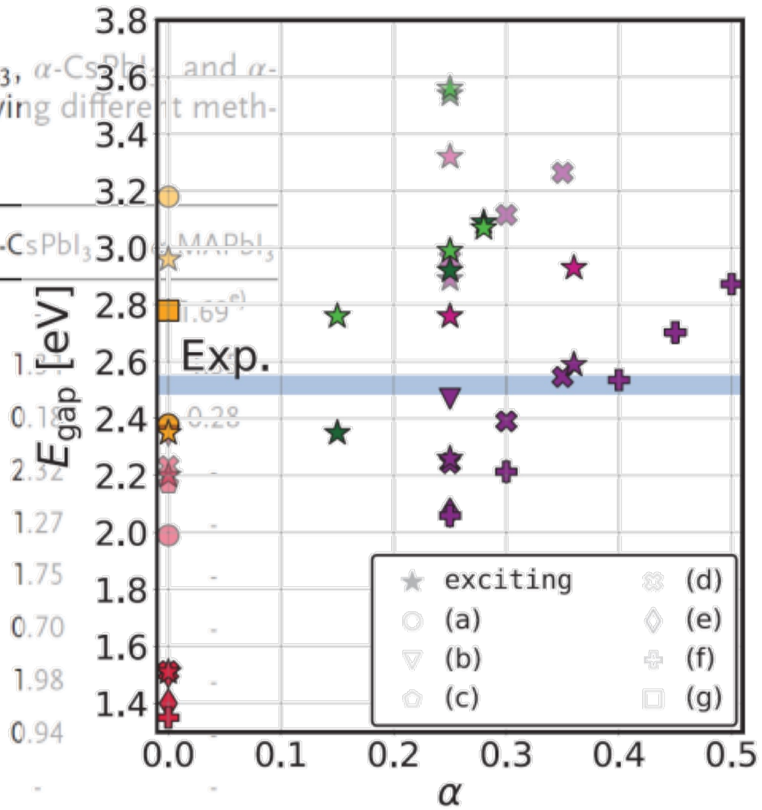
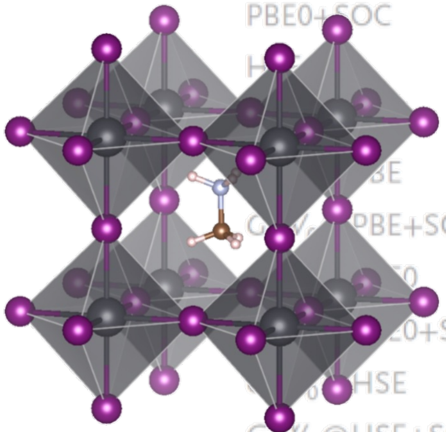


Table 1. Electronic band gaps (in eV) of PbI_2, γ-$CsPbI_3$, α-$CsPbI_3$ and α-$MAPbI_3$, calculated with and without SOC and employing different methods.

	PbI_2	γ-$CsPbI_3$	α-$CsPbI_3$	$MAPbI_3$
Exp.	2.55[a], 2.485[b]	1.73[c], 1.67[d]		1.69[e]
PBE	2.20	1.58	[illegible]	[illegible]
PBE+SOC	1.51	0.63	0.18	0.28
PBE0	3.54	2.75	2.32	-
PBE0+SOC	2.92	1.86	1.27	-
[illegible]	2.89	2.13	1.75	-
[illegible]	2.26	1.25	0.70	-
[illegible]	2.96	2.17	1.98	-
G_0W_0@PBE+SOC	2.35	1.32	0.94	-
[illegible]	3.56	2.84	-	-
[illegible]	2.99	1.99	-	-
[illegible]	3.32	2.54	-	-
G_0W_0@HSE+SOC	[illegible]	[illegible]	-	-

a) Ref. [22]; b) ref. [23]; c) refs. [75, 76]; d) ref. [[77]]; e) ref. [73].





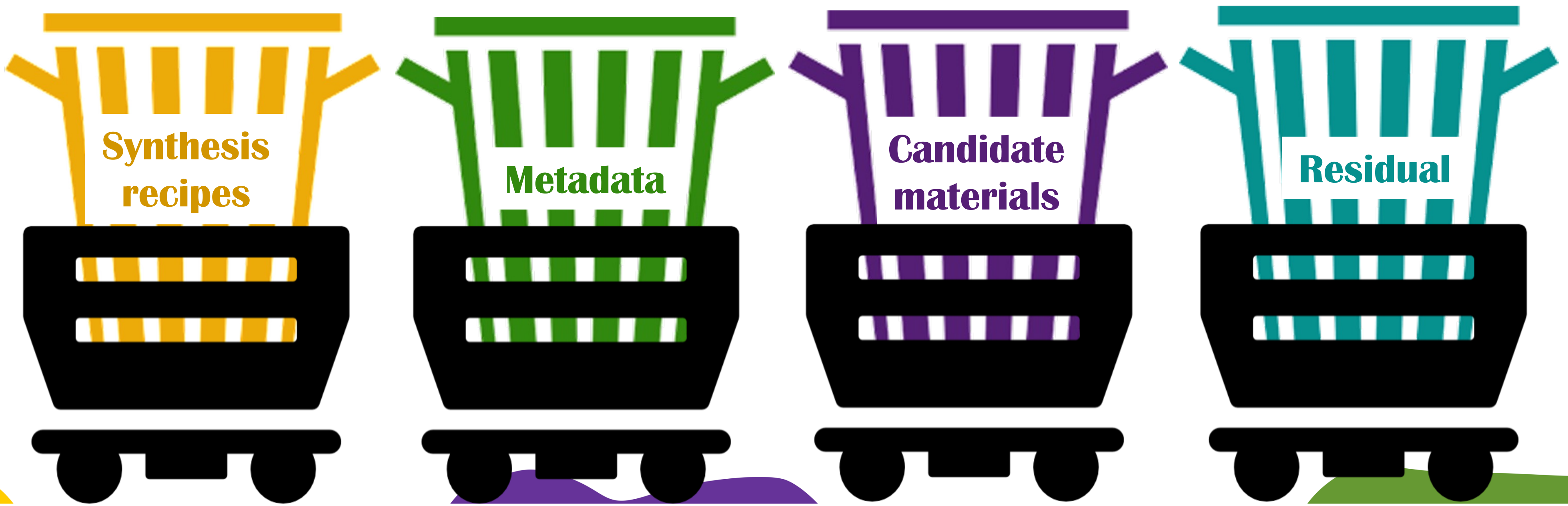
We never provide all information!

Let's keep recycling ...

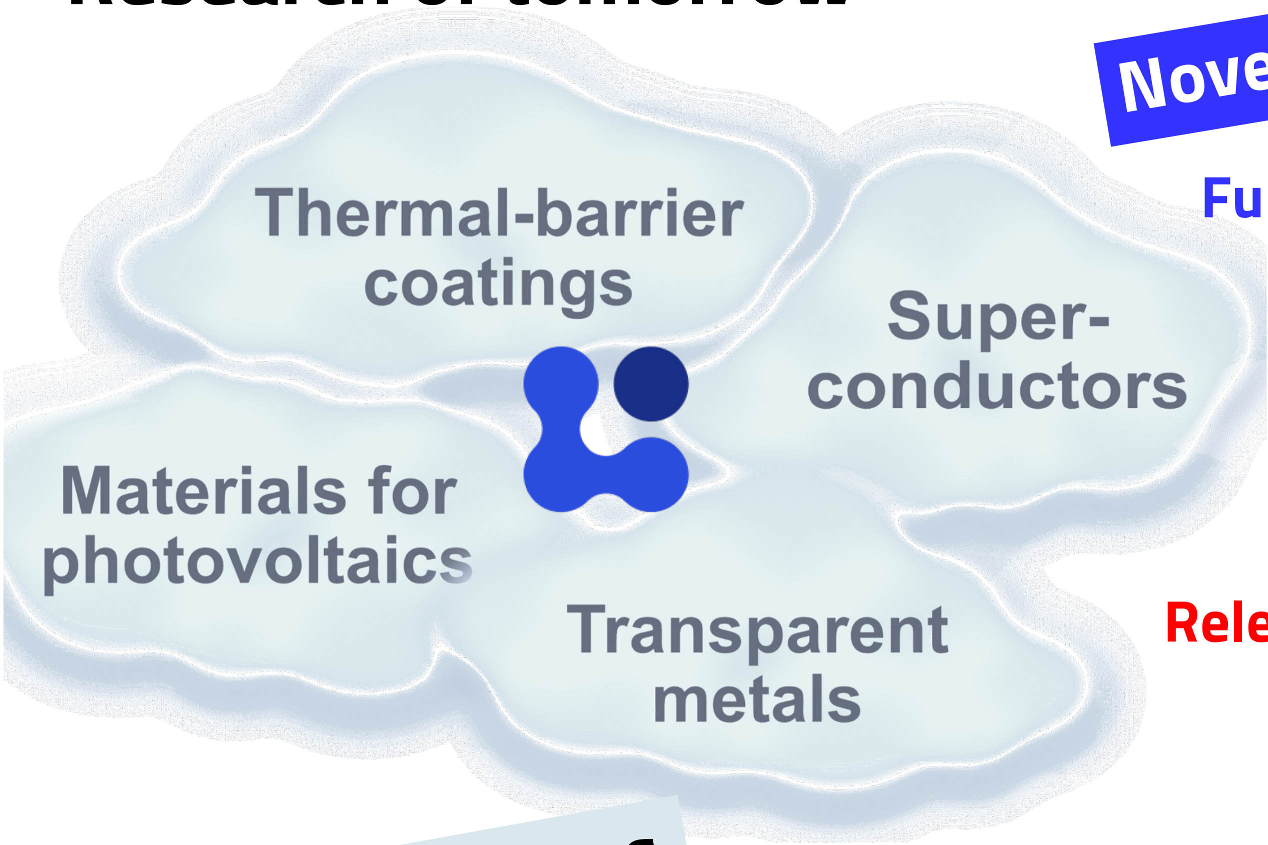
Need to learn from failures	Only annoted data can be reused	Bad for one, good for another purpose	Carry lots of knowledge
Synthesis recipes	Metadata	Candidate materials	Residual
Apparently not successful	(Handwritten) labbooks	Not useful for purpose-oriented research	Not used in publications

Raw material of the 21st century

Turn trash into a gold mine!



Research of tomorrow



Trends & patterns

Novel tools

Beyond interpolation

Fully documented, published models

The right data

Relevant, high-quality data

The exceptional

A bit of history

2011

Office of Science and Technology Policy

About OSTP | Pressroom | OSTP Blog | Divisions | Initiatives | R&D Budgets | Resource

"To help businesses discover, develop, and deploy new materials twice as fast, we're launching what we call **the Materials Genome Initiative**.

The invention of silicon circuits and lithium ion batteries made computers and iPods and iPads possible, but it took years to get those technologies from the drawing board to the market place. **We can do it faster.**"

-President Obama (6/11)

2015

It's Time to Open Materials Science Data

Posted by Cyrus Wadia and Michael Stebbins

Feb 6, 2015:

"... That data underlying scientific publications are not available for confirmatory analysis, reuse, and repurposing is an anachronism that we aim to address. ..."

a. The materials-research
STP-, NSF-, and
h larger scale of materials
and hosted by the Materials
mendous opportunities to innovate with open data. Federal agencies have also stepped up to
aterials community, including the Materials Project for novel batteries, DOE's hydrogen
LOWLIB.org repository for quantum materials.

2016

scientific **data**

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nature > scientific data > comment > article

Comment | Open access | Published: 15 March 2016

The FAIR Guiding Principles for scientific data management and stewardship

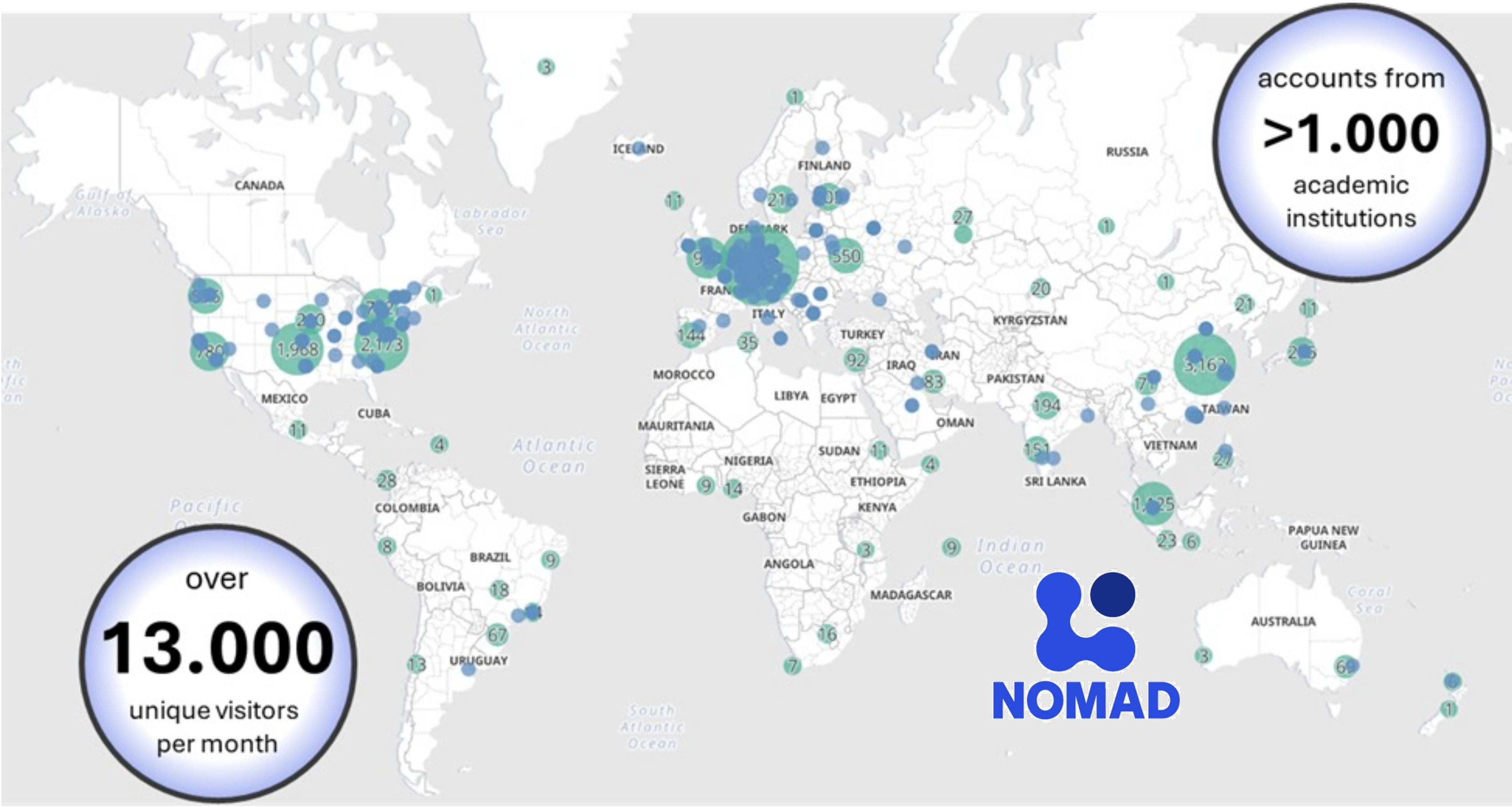
Mark D. Wilkinson, Michel Dumontier, IJsbrand Jan Aalbersberg, Gabrielle Appleton, Myle
Baak, Niklas Blomberg, Jan-Willem Boiten, Luiz Bonino da Silva Santos, Philip E. Bourne, J
Anthony J. Brookes, Tim Clark, Mercè Crosas, Ingrid Dillo, Olivier Dumon, Scott Edmunds,
Richard Finkers, Alejandra Gonzalez-Beltran, Alasdair J.G. Gray, Paul Groth, Carole Goble,
... Barend Mons + Show authors

Scientific Data **3**, Article number: 160018 (2016) | Cite this article

A bit more of history ...

C. Draxl and M. Scheffler, MRS Bulletin 43, 676 (2018); J. Phys. Mater. 2, 036001 (2019).

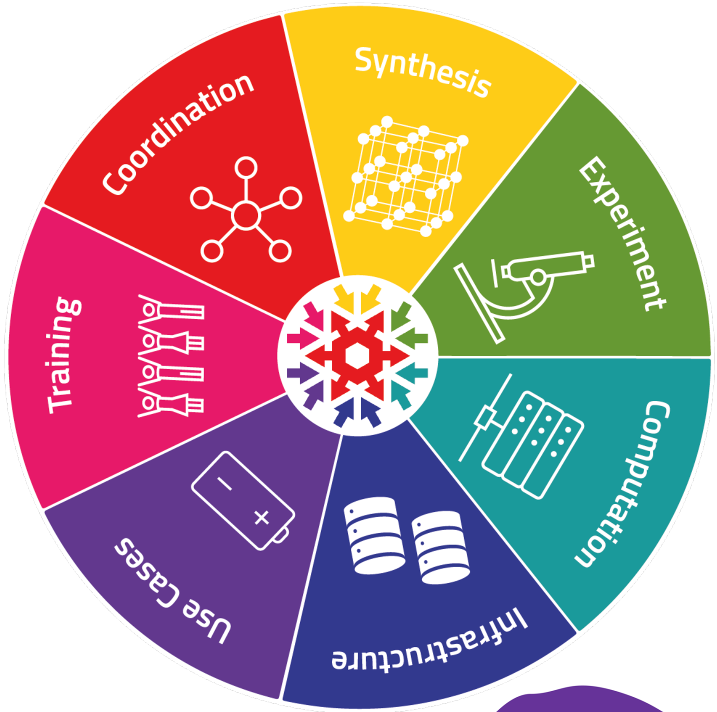
Institutions with registered users



More FAIRness ....

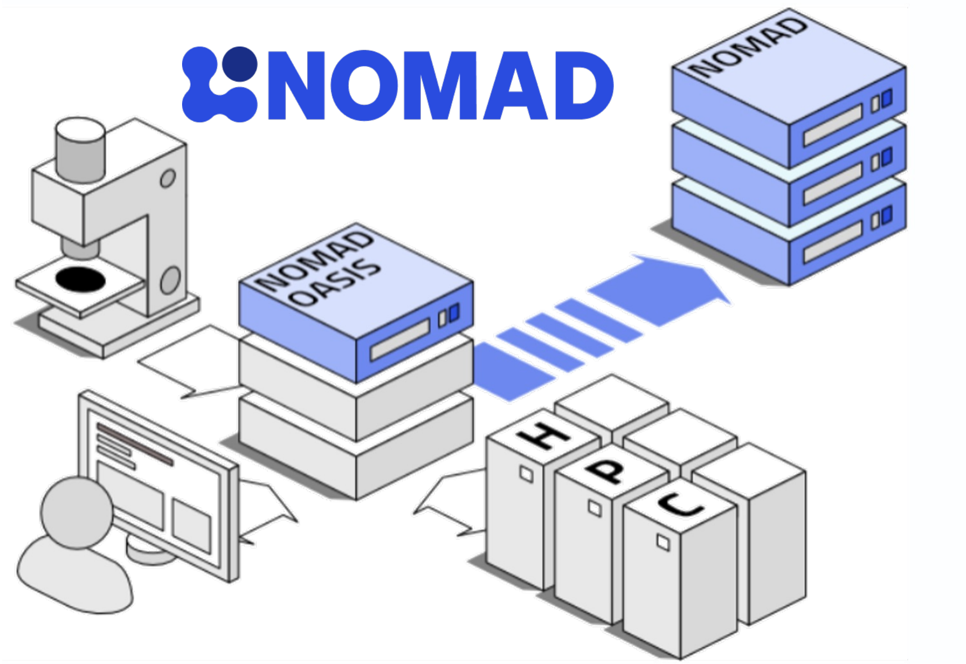
FAIRmat is the NFDI consortium for solid state physics and the chemical physics of solids

https://fairmat-nfdi.eu



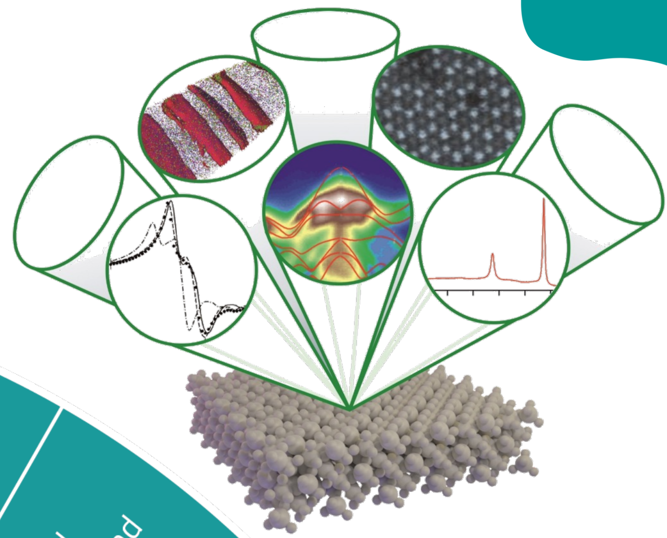
NOMAD is a web-based software for FAIR research data management in materials science

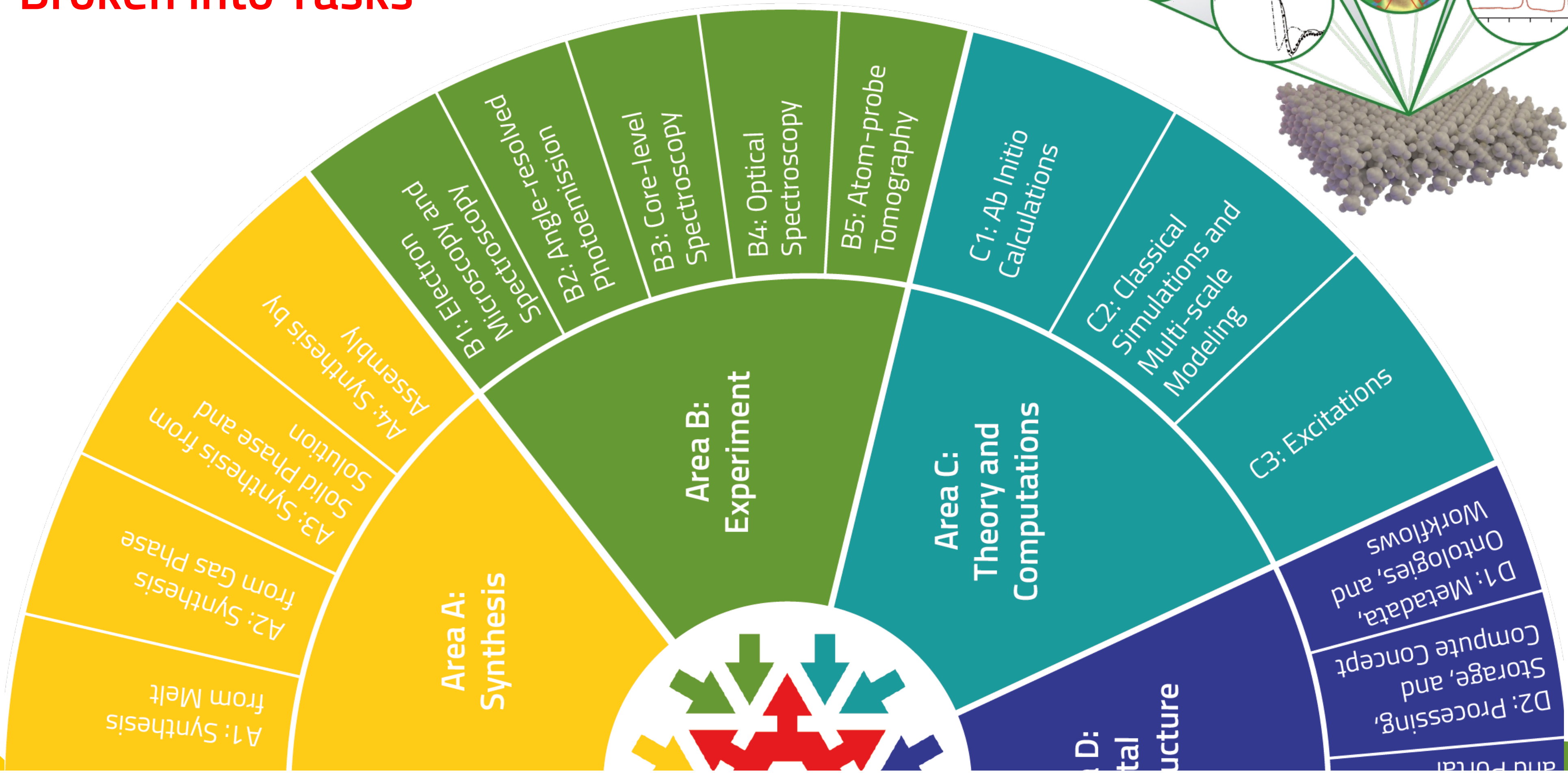
https://nomad-lab.eu

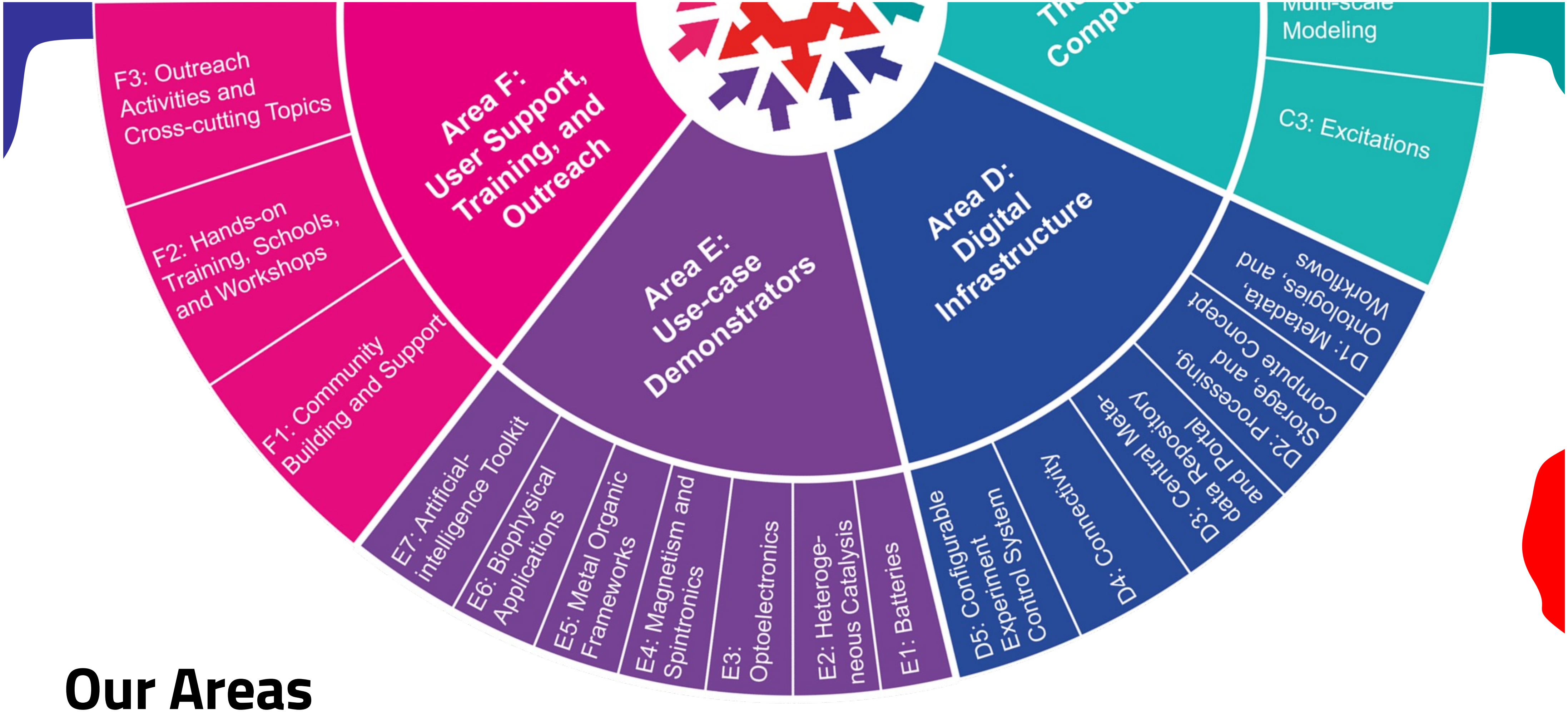


Our Areas

Broken into Tasks





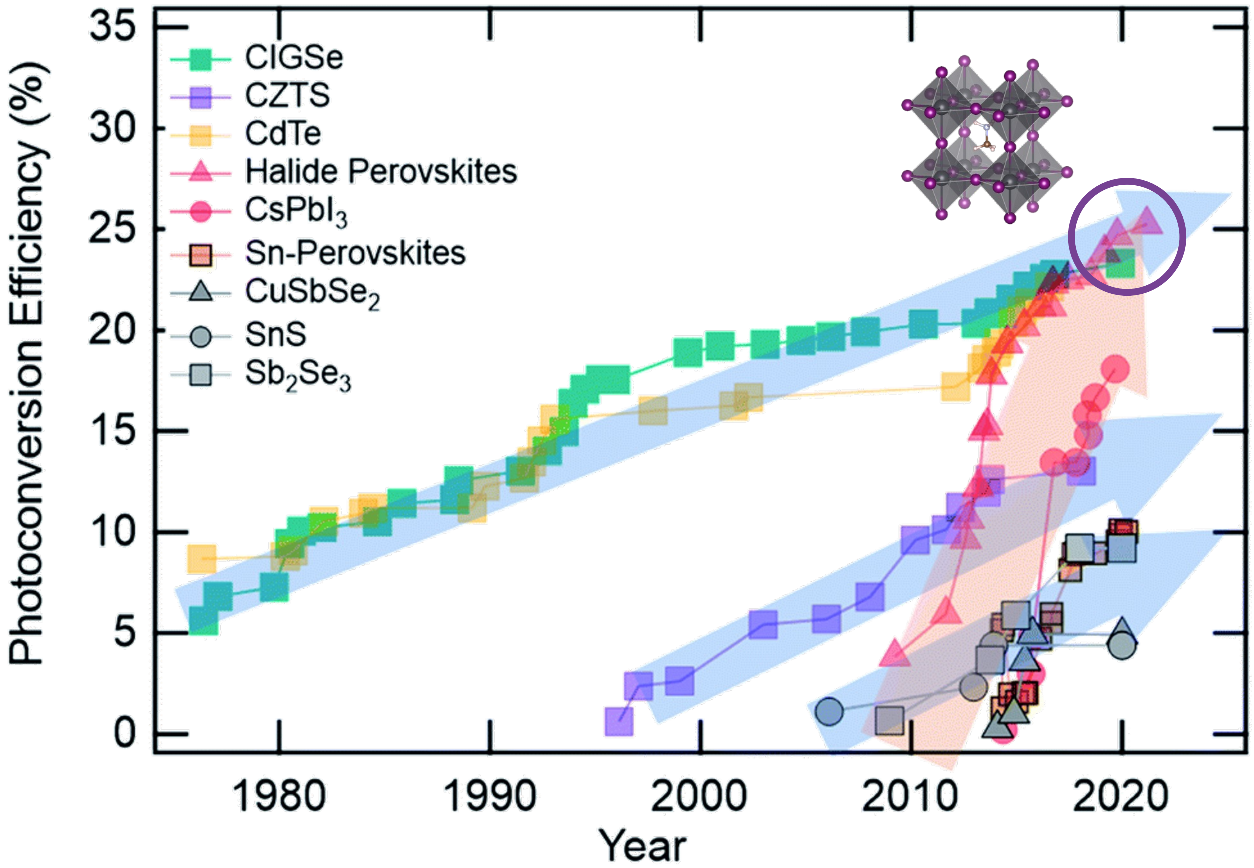


Our Areas

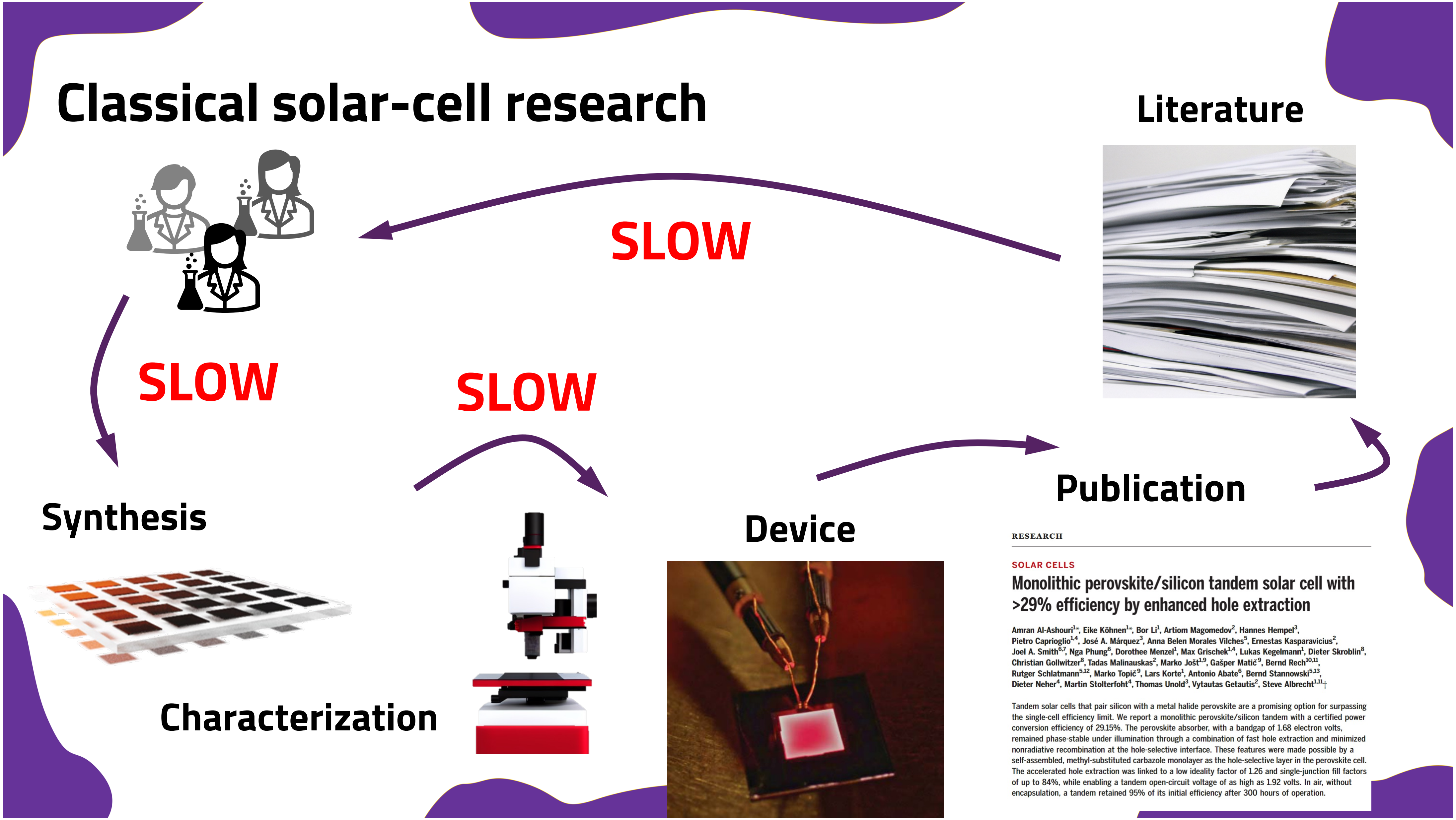
Broken into Tasks

A specific example

A long way to the roof ...

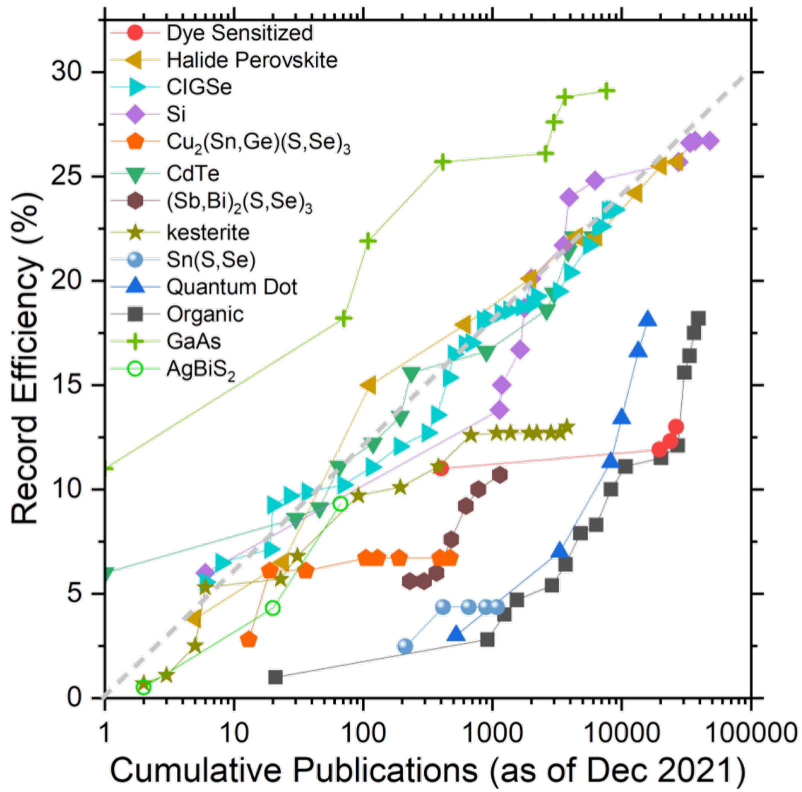


T. Unold, Faraday Discuss. 239, 235 (2022).



Classical solar-cell research
Literature
SLOW
SLOW
SLOW
Synthesis
Characterization
Device
Publication
RESEARCH
SOLAR CELLS
Monolithic perovskite/silicon tandem solar cell with >29% efficiency by enhanced hole extraction
Amran Al-Ashouri[1]*, Eike Köhnen[1]*, Bor Li[1], Artiom Magomedov[2], Hannes Hempel[3], Pietro Caprioglio[1,4], José A. Márquez[3], Anna Belen Morales Vilches[5], Ernestas Kasparavicius[2], Joel A. Smith[6,7], Nga Phung[6], Dorothee Menzel[1], Max Grischek[1,4], Lukas Kegelmann[1], Dieter Skroblin[8], Christian Gollwitzer[8], Tadas Malinauskas[2], Marko Jošt[1,9], Gašper Matič[9], Bernd Rech[10,11], Rutger Schlatmann[5,12], Marko Topič[9], Lars Korte[1], Antonio Abate[6], Bernd Stannowski[5,13], Dieter Neher[4], Martin Stolterfoht[4], Thomas Unold[3], Vytautas Getautis[2], Steve Albrecht[1,11]†
Tandem solar cells that pair silicon with a metal halide perovskite are a promising option for surpassing the single-cell efficiency limit. We report a monolithic perovskite/silicon tandem with a certified power conversion efficiency of 29.15%. The perovskite absorber, with a bandgap of 1.68 electron volts, remained phase-stable under illumination through a combination of fast hole extraction and minimized nonradiative recombination at the hole-selective interface. These features were made possible by a self-assembled, methyl-substituted carbazole monolayer as the hole-selective layer in the perovskite cell. The accelerated hole extraction was linked to a low ideality factor of 1.26 and single-junction fill factors of up to 84%, while enabling a tandem open-circuit voltage of as high as 1.92 volts. In air, without encapsulation, a tandem retained 95% of its initial efficiency after 300 hours of operation.

Classical solar-cell research



Literature

P. Dale and M. A. Scarpulla, Sol. Energy Mater. Sol. Cells (2023).

The Perovskite Database Project

Pioneering project

100 authors

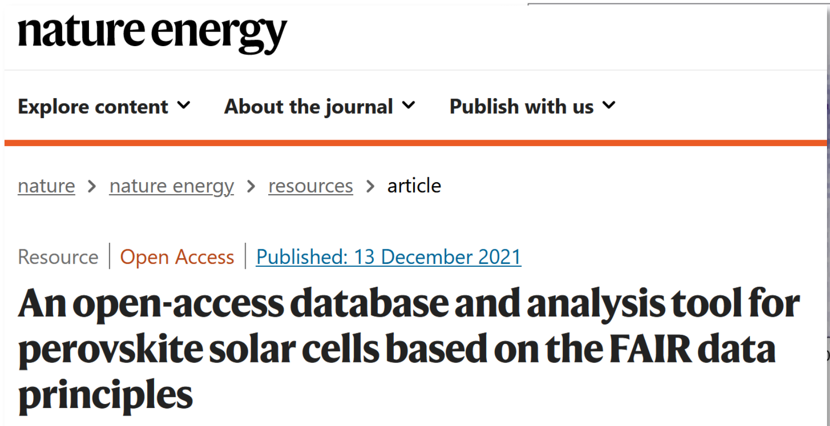
Manual handling of

- 42 000 devices
- 16 000 publications

More than 400 metadata categories

Synthesis information

Difficult to update


nature energy

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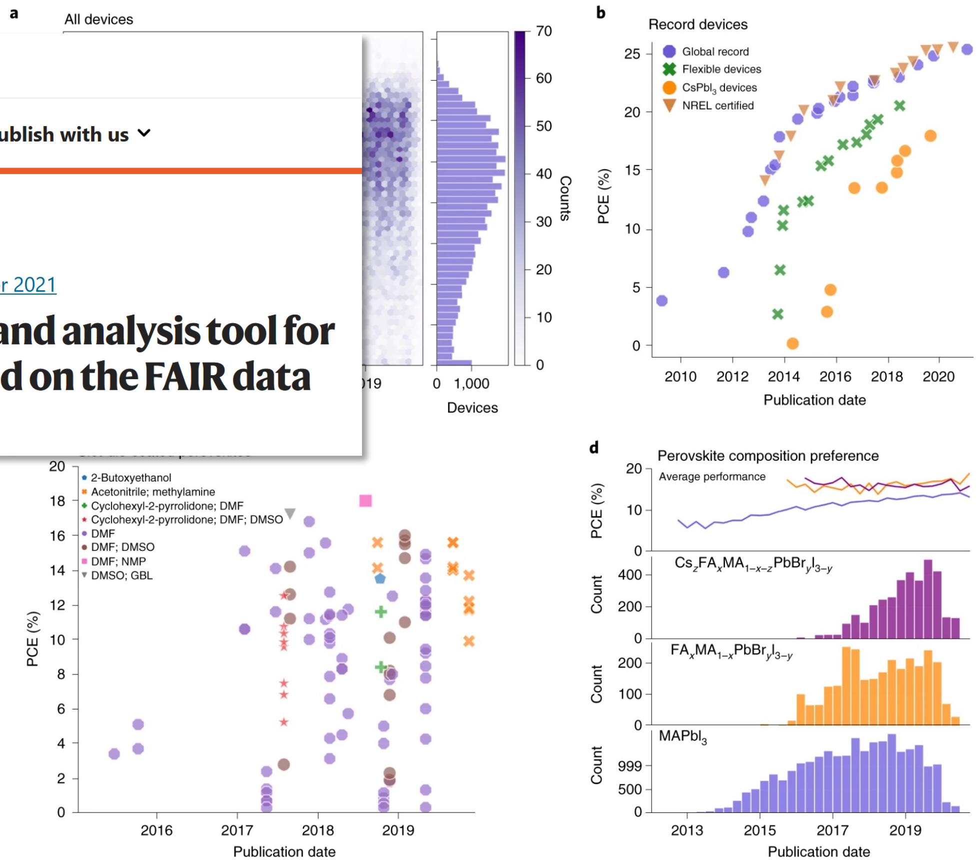
Resource | Open Access | Published: 13 December 2021

An open-access database and analysis tool for perovskite solar cells based on the FAIR data principles



J. Jacobsson, et al. Nature Energy 7, 107 (2022).

Heterogenous sources

Efficiency tables

TOPICAL REVIEW • OPEN ACCESS

Emerging inorganic solar cell efficiency tables (version 2)

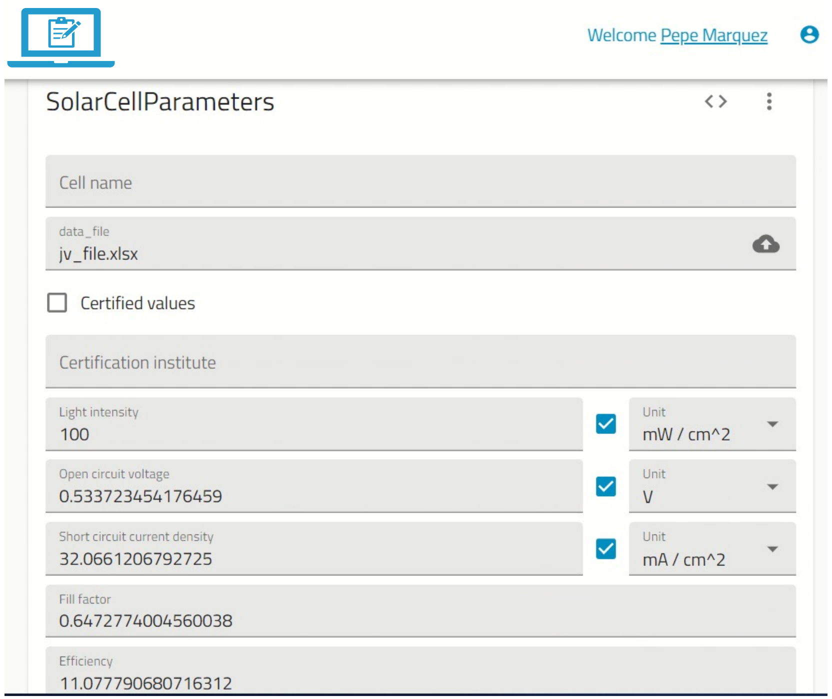
Andriy Zakutayev[1], Jonathan D Major[2], Xiaojing Hao[3], Aron Walsh[4,5], Jiang Tang[6], Teodor K Todorov[7], Lydia H Wong[8] and Edgardo Saucedo[10,9]

Published 16 April 2021 • © 2021 The Author(s). Published by IOP Publishing Ltd

Journal of Physics: Energy, Volume 3, Number 3

Citation Andriy Zakutayev *et al* 2021 *J. Phys. Energy* **3** 032003

Lab notebooks



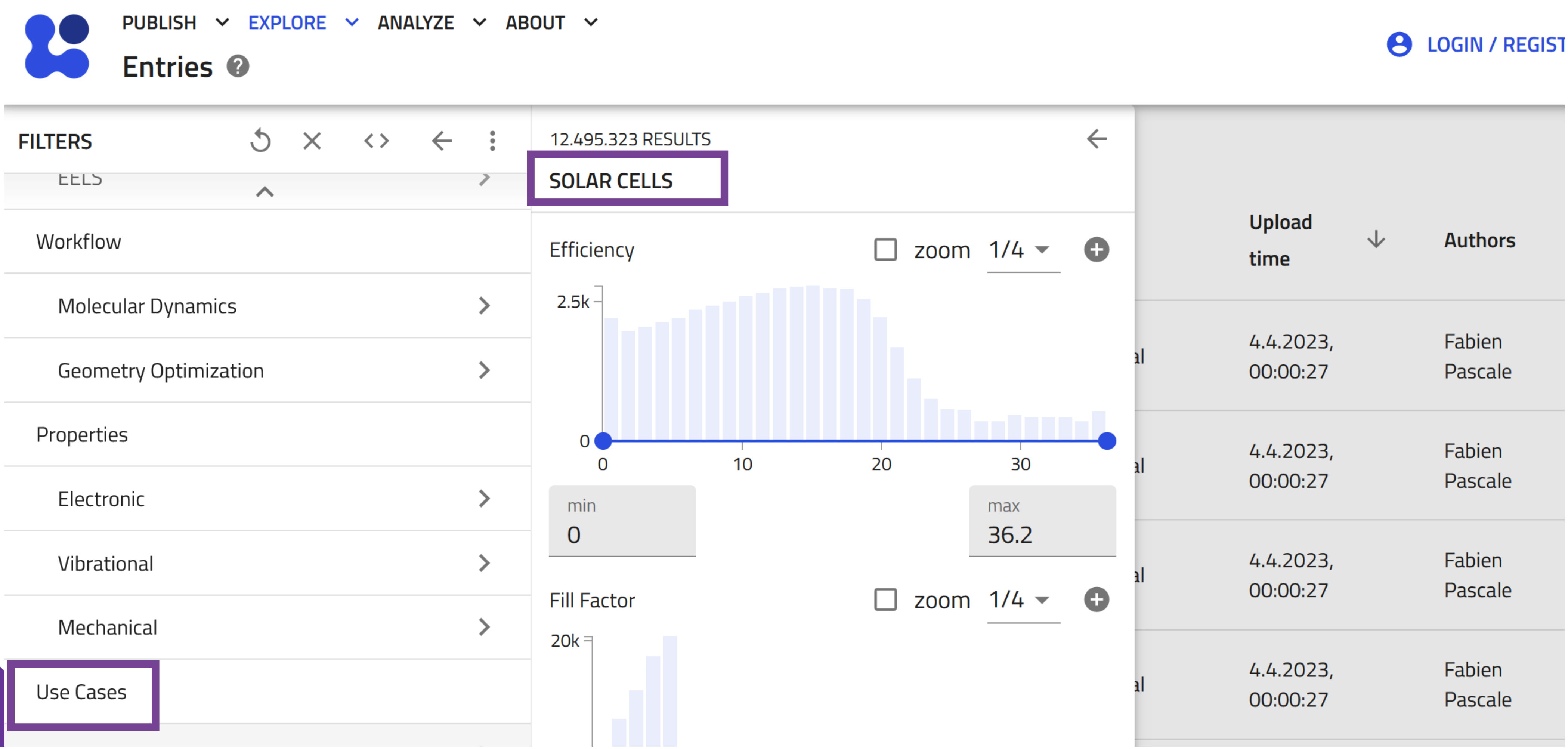
Databases

EMERGING PV

The Perovskite database

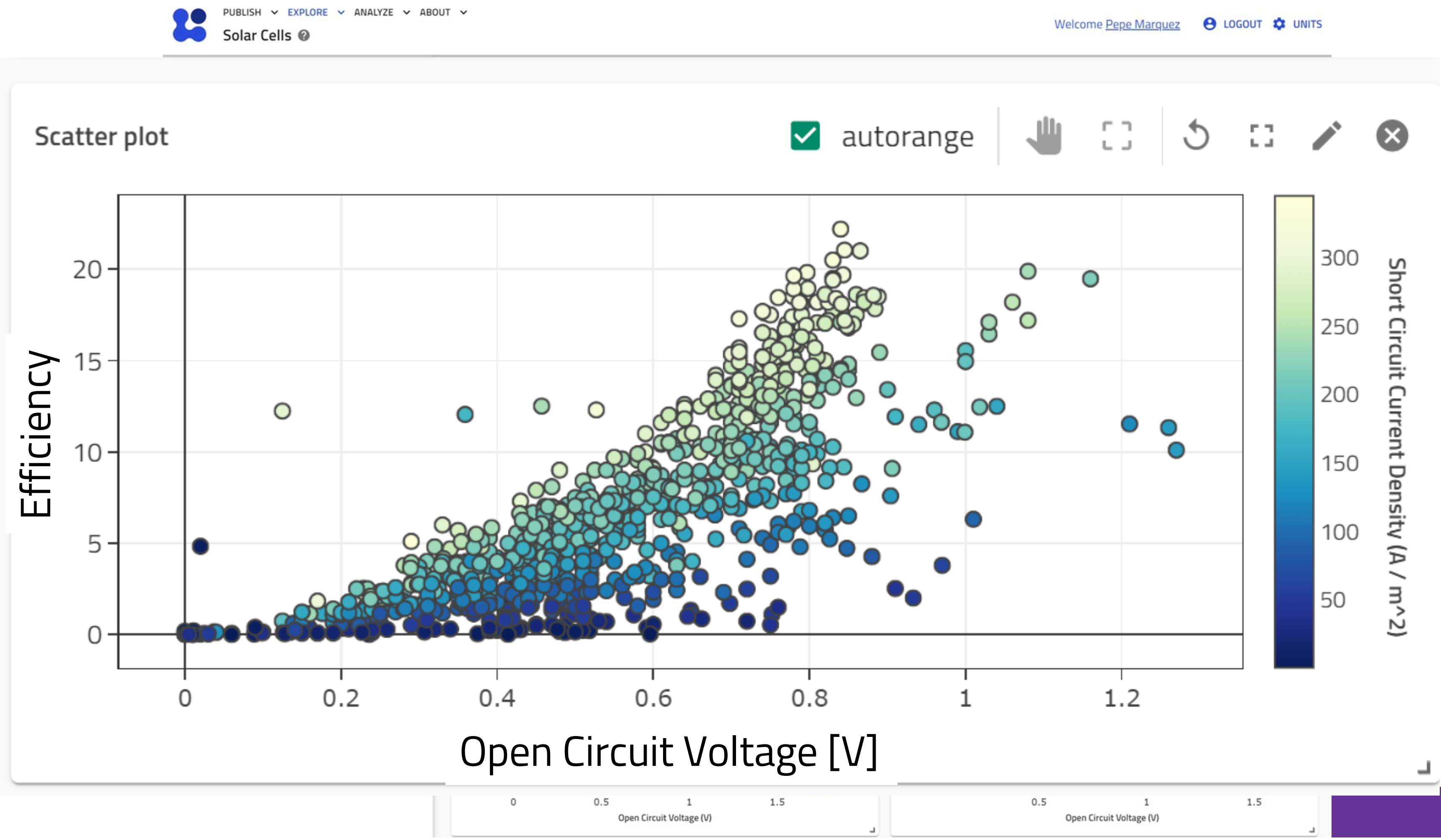
https://nomad-lab.eu

Explore solar cells in NOMAD



https://nomad-lab.eu

Explore solar cells in NOMAD

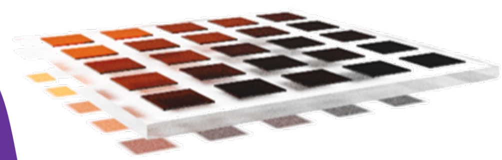


P. Marquez

Local data infrastructure

SLOW

Synthesis



Characterization

Combinatorial synthesis

High throughput characterization

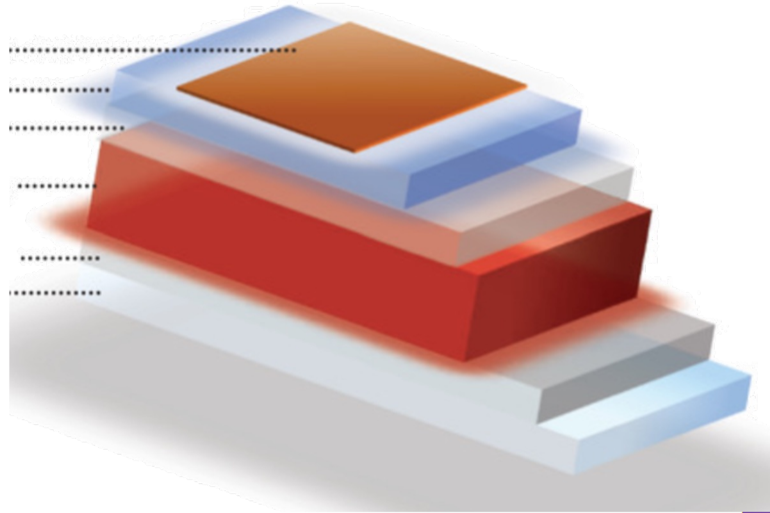
Autonomous labs

AI support

NOMAD OASIS

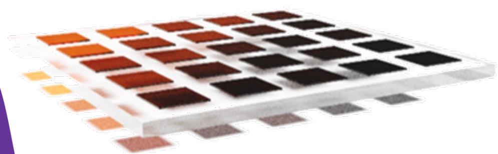
Combinatorial explosion

Device stack



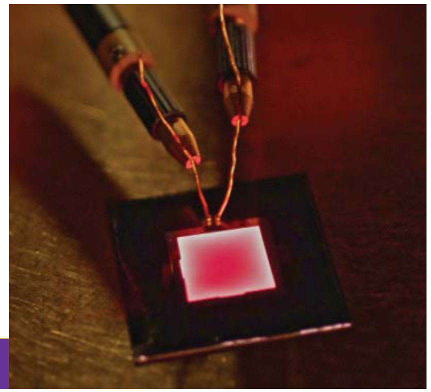
SLOW

Synthesis



Characterization

Device



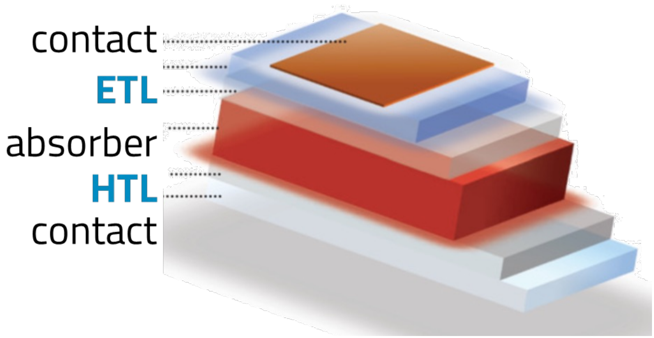
ETL: electron transport layer

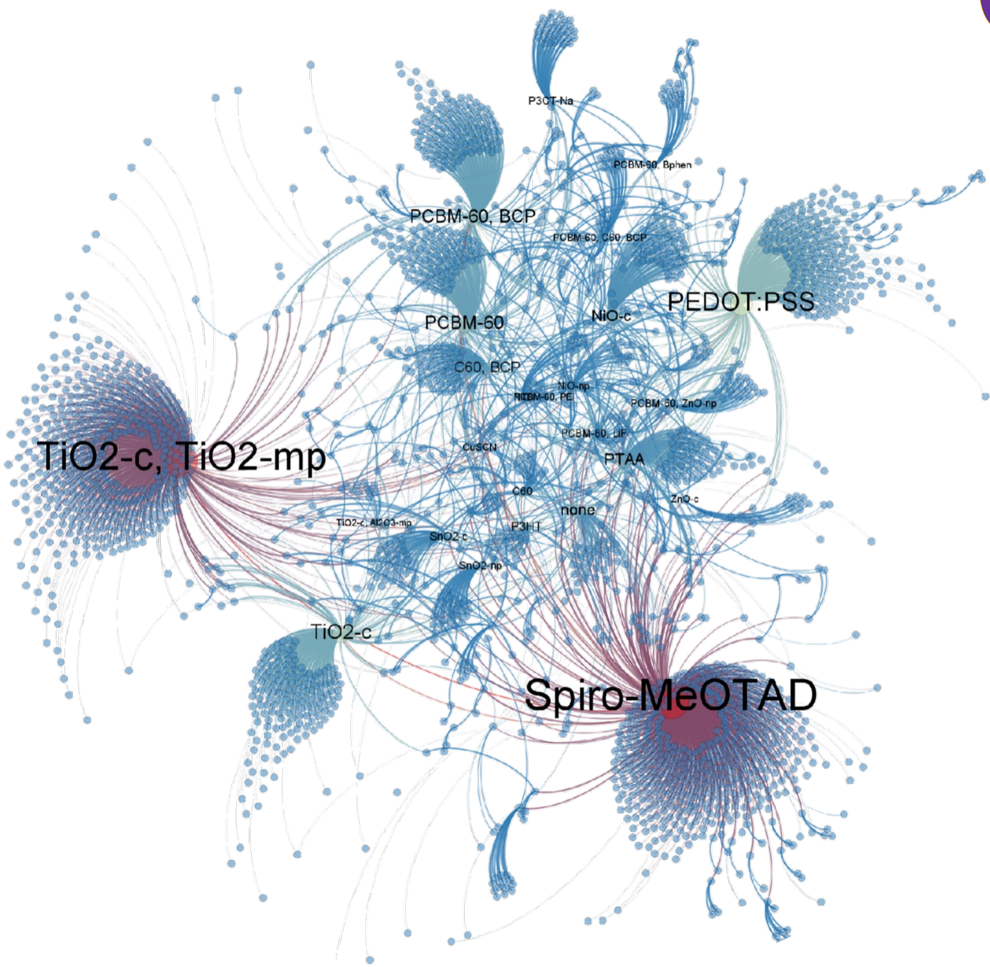
HTL: hole transport layer

Device stack

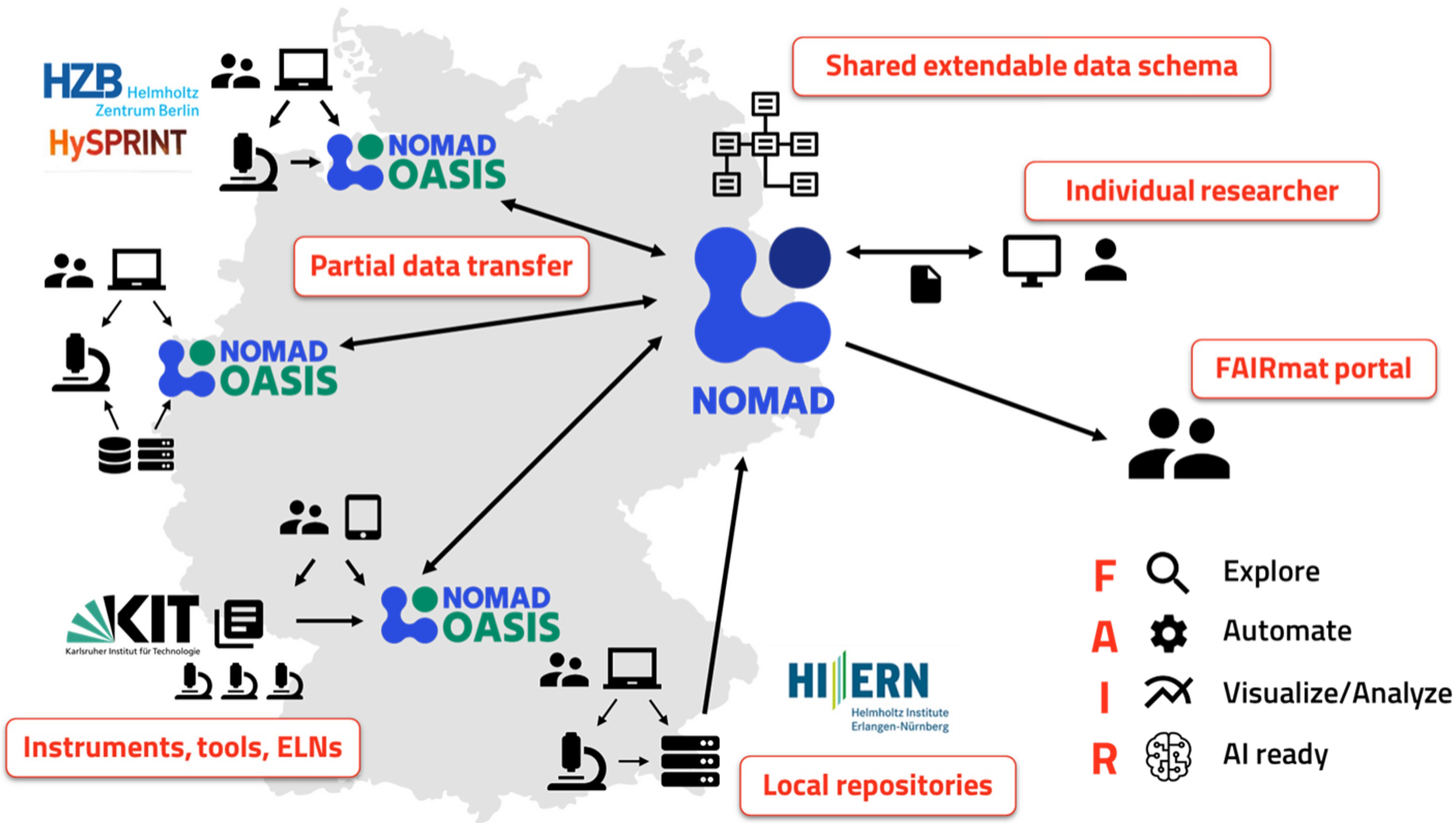
2600 nodes

Charge transport layers





A Solar Network



Back to data infrastructure

5. M. Scheffler, M. Aeschlimann, M. Albrecht, T. Bereau, H.-J. Bungartz, C. Felser, M. Greiner, A. Groß, C. Koch, K. Kremer, W. E. Nagel, M. Scheidgen, C. Wöll, and C. Draxl
FAIR data enabling new horizons for materials research
Nature **604**, 635 (2022). [DOI] [arXiv]

JOSS
The Journal of Open Source Software

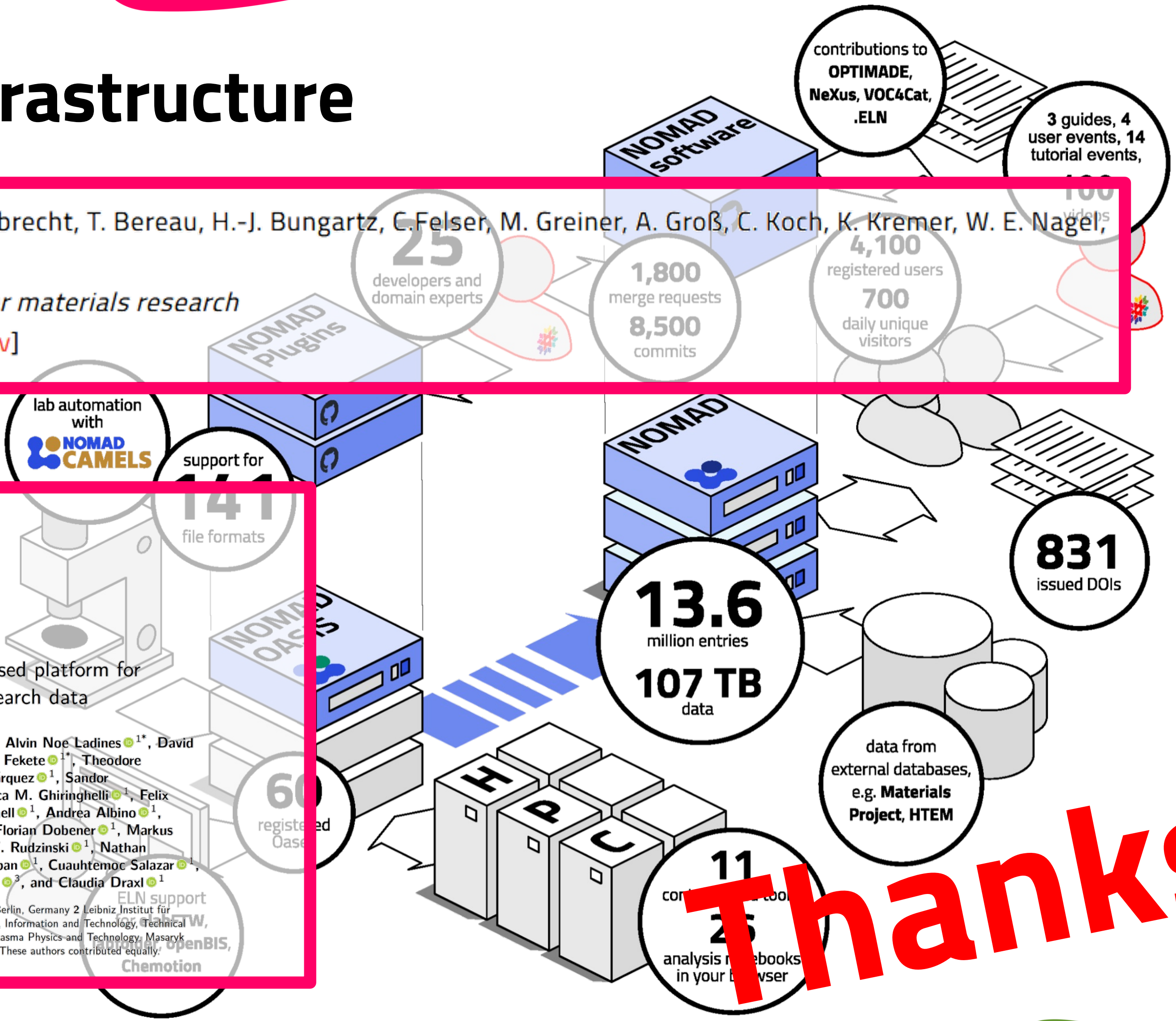
NOMAD: A distributed web-based platform for managing materials science research data

Markus Scheidgen[1*¶], Lauri Himanen[1*], Alvin Noe Ladines[1*], David Sikter[1*], Mohammad Nakhaee[1*], Ádám Fekete[1*], Theodore Chang[1*], Amir Golparvar[1*], José A. Márquez[1], Sandor Brockhauser[1], Sebastian Brückner[2], Luca M. Ghiringhelli[1], Felix Dietrich[3], Daniel Lehmberg[3], Thea Denell[1], Andrea Albino[1], Hampus Näsström[1], Sherjeel Shabih[1], Florian Dobener[1], Markus Kühbach[1], Rubel Mozumder[1], Joseph F. Rudzinski[1], Nathan Daelman[1], José M. Pizarro[1], Martin Kuban[1], Cuauhtemoc Salazar[1], Pavel Ondračka[4], Hans-Joachim Bungartz[3], and Claudia Draxl[1]

1 Department of Physics, Humboldt-Universität zu Berlin, Berlin, Germany 2 Leibniz Institut für Kristallzüchtung, Berlin, Germany 3 School of Computation, Information and Technology, Technical University of Munich, Munich, Germany 4 Department of Plasma Physics and Technology, Masaryk University, Brno, Czech Republic ¶ Corresponding author * These authors contributed equally.

DOI: 10.21105/joss.05388

JOSS 8, 5388 (2023).



Thanks!!