HZB Helmholtz Zentrum Berlin

HySPRINT Helmholtz Innovation Lab

VIPERLAB workshop
8th Feb 2022 ONLINE

The Perovskite Database: The United Output of the Perovskite PV community

Dr. Jesper Jacobsson

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GRECO

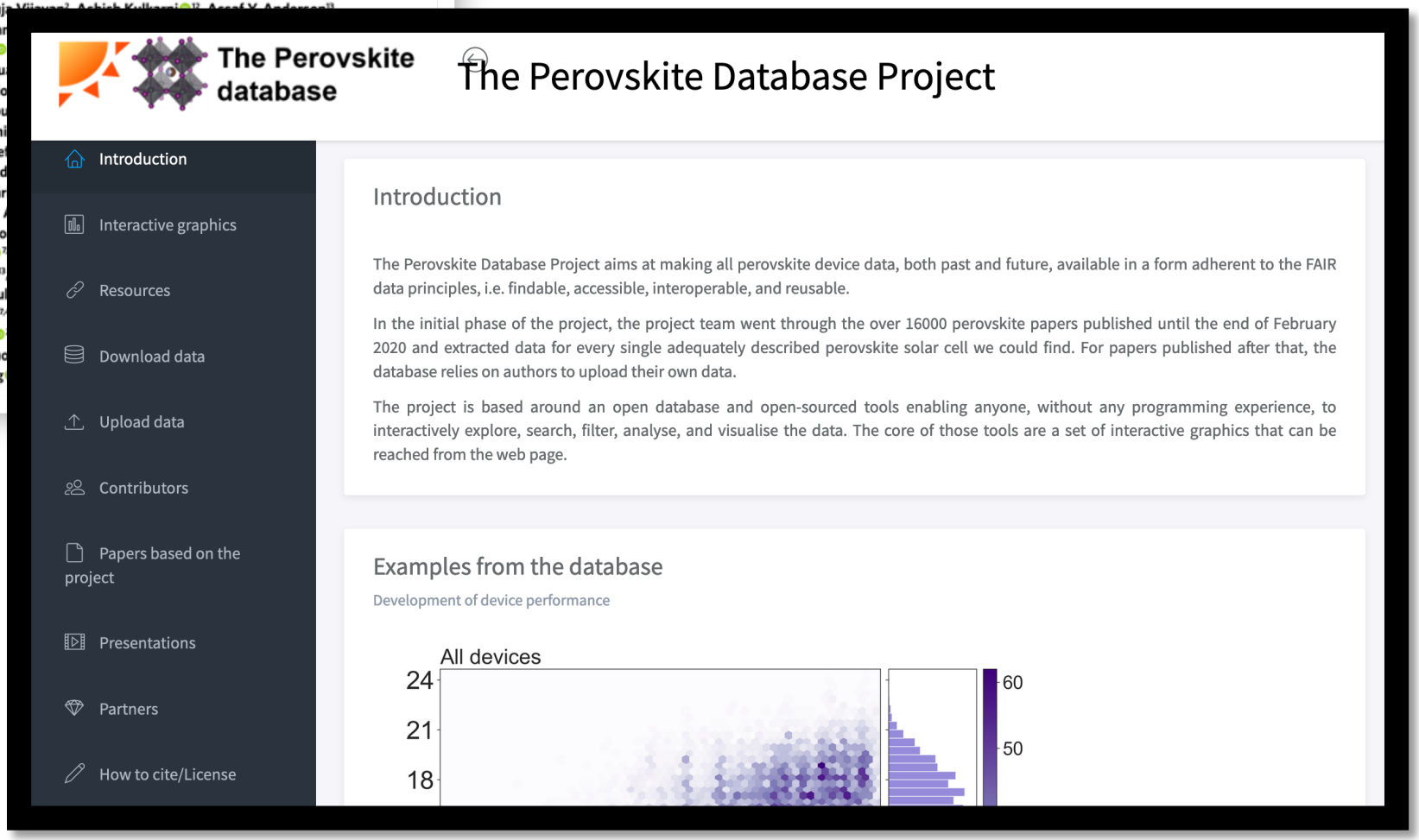
VIPERLAB

Initiated as part of the EU-funded project GRECO

Release article:

Jacobsson et al., Nature Energy 2021
(DOI: 10.1038/s41560-021-00941-3)

Project webpage: www.perovskitedatabase.com



Initiated as part of the EU-funded project GRECO

GRECO *”bringing open science into action”*

“Open Research Europe **requires open access** to **research data** supporting articles under the principle ‘as open as possible, as closed as necessary’, according to the policy of Horizon 2020. **Data should be deposited in data repositories**.”

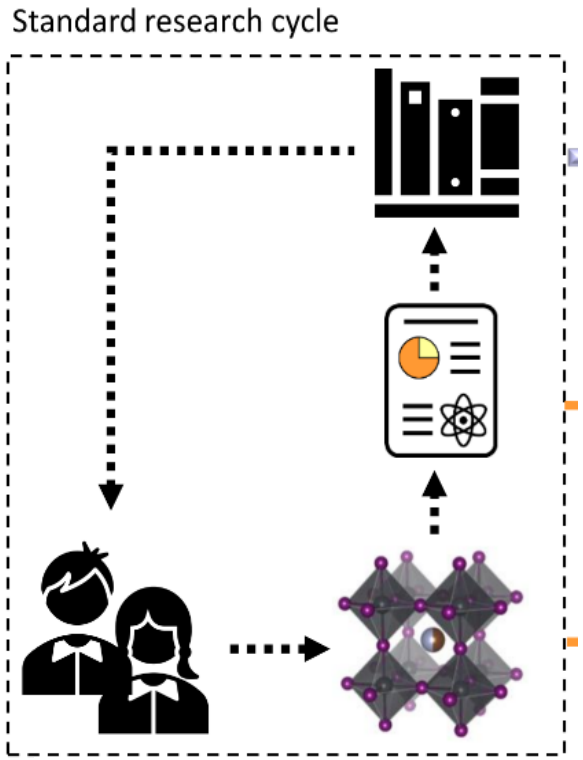
from: https://open-research-europe.ec.europa.eu/for-authors/data-guidelines

What are suitable repositories? – existing ones mostly ”generic”

What would be data platforms that are actually useful for us scientist that
Truly make our results more FAIR (findable, accessible, interoperable & reusable)?

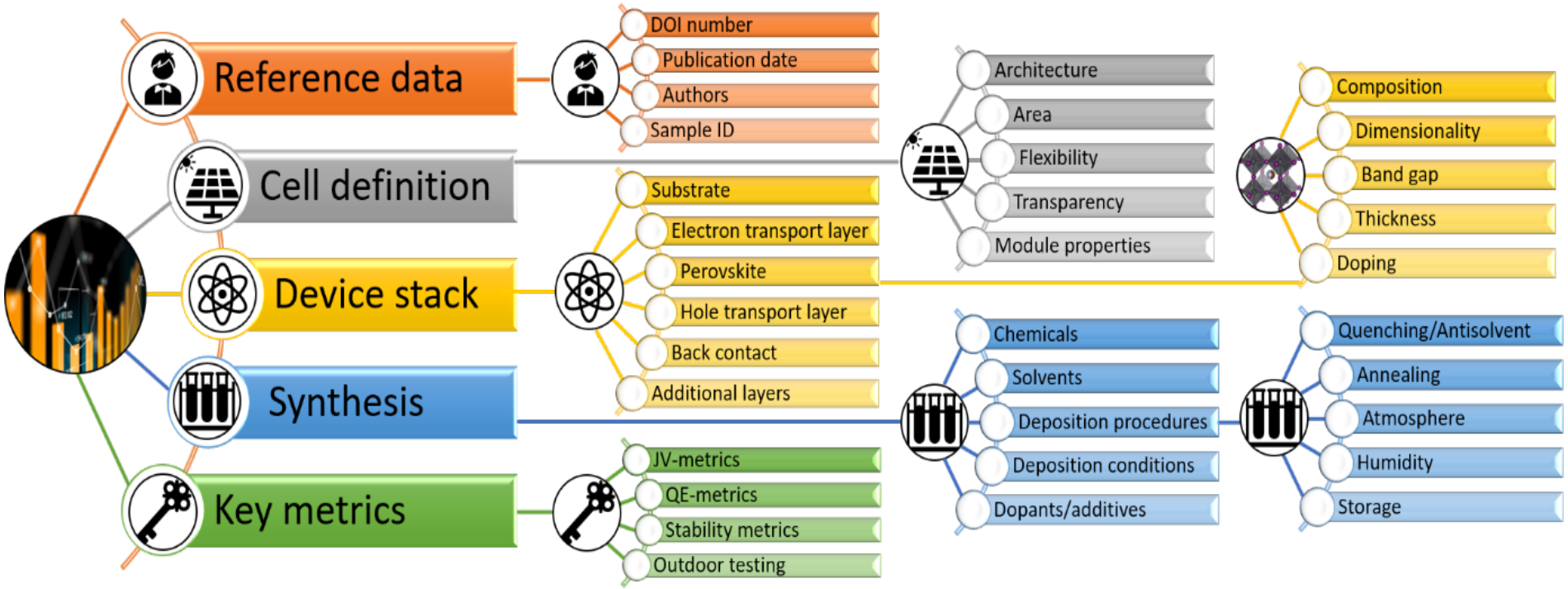
This project was funded as part of the GRECO project, funded by the European Union’s Horizon 2020 research and innovation program under grant agreement No. 787289.

The motivation: Breaking the ”standard research cykle”



Step 1: Defining the ”data ontology” (first draft)

Focussed on meta-data related to device stack definition & solar cell performance



There is a need to develop coherent data ontologies
to speficify metadata of device manufacturing steps.

VIPERLAB

Major goal of VIPERLAB:
Develop a unified data ontology for perovskite PV devices.
(there will be a workshop…)

Data extraction protocol (current version available online)

The Perovskite database

The Perovskite Database Project

- Introduction
- Interactive graphics
- Resources
- Download data
- Upload data
- Contributors
- Papers based on the project
- Presentations
- Partners
- How to cite/License

More data makes the database m

The database was initiated by collecting all perc
community should embrace this as a valuable re
can think of as the Wikipedia of perovskite scien

We thus encourage anyone to upload new devic
highly efficient or a failed device, but some data

Data extraction protocol

To upload new data to the database, the data m
backend for inserting data to the database cons
formatting guidelines. The latest version of the
template are found in the template. The instruct

Download data extraction template

Download data extraction instructions

Current version:
395 attributes/fields
per devices (and growing)

	A	B
1	Ref. ID temp (Integer starting from 1 and counting upwards)	1
2	Ref. Name of person entering the data	T. Jesper Jacobsson
3	Ref. Data entered by author [TRUE/FALSE]	TRUE
4	Ref. DOI number	10.1039/C6EE00030D
5	Ref. Lead author	Jacobsson et al.
6	Ref. Publication date [year:mm:dd]	2018:03:14
7	Ref. Free text comment (max 280 characters)	Simple example device (to be deleated)
8	Ref. Internal sample ID [free text]	JJ 3051 cell 2
9	Cell. Stack sequence [Mat.1; Mat.2; ... | Mat.3; ... | Mat.4 | ...]	SLG | FTO | TiO2-c | TiO2-mp | Perovskite | Spiro-MeOTAD | Au
10	Cell. Area. Total [cm^2]	0,25
11	Cell. Area. Measured [cm^2]	0,16
12	Cell. Number of cells per substrate	3
13	Cell. Architecture [nip/pin/ ...]	nip
14	Cell. Flexible [TRUE/FALSE]	FALSE
15	Cell. Flexible. Minimum bending radius [cm]	
16	Cell. Semitransparent [TRUE/FALSE]	FALSE
17	Cell. Semitransparent. Average visible transmittance [%]	
18	Cell. Semitransparent. Average visible transmittance. Wavelength range [lambda_min; lambda_max]	
19	Cell. Semitransparent. Transmittance. Link. Raw data	www.testsite...
20	Module [TRUE/FALSE]	FALSE
21	Module. Number of cells in module	0
22	Module. Area. Total [cm^2]	0,25
23	Module. Area. Effective [cm^2]	0,16
24	Module. JV data recalculated per cell [TRUE/FALSE]	FALSE
25	Substrate. Stack sequence [Mat.1; Mat.2; ... | Mat.3; ... | Mat.4 | ...]	SLG | FTO
26	Substrate. Thickness [Th.1 | Th.2 | ... | Th.n] [mm]	2 | 0.1
27	Substrate. Area [cm^2]	2,4
28	Substrate. Supplier	NGO
29	Substrate. Brand name	NGO11
30	Substrate. Deposition procedure [Proc. 1 >> Proc. 2 >> ... | Proc. 3 >> ...	Commercial | Commercial
31	Substrate. Surface roughness. Rms [nm]	
32	Substrate. Etching procedure	Zn-powder; HCl >> Mecanical scrubbing
33	Substrate. Cleaning procedure	Helmanex >> Ultrasonic bath >> Ethanol; Ultrasonic bath >> Acetone; Ultrasonic
34	ETL. Stack sequence [Mat.1; Mat.2; ... | Mat.3; ... | Mat.4 | ...]	TiO2-c | TiO2-mp
35	ETL. Thickness [Th.1 | Th.2 | ... | Th.n] [nm]	50 |150
36	ETL. Additives. Compounds [Addt.1; Addt.2; ... | Addt.3; ... | Addt.4 | ...	Undoped | Li-TFSI
37	ETL. Additives. Concentrations [c1 M; c2 wt%; ... | c3 vol%; ... | c4 mg/m	nan | 100 mg/ml
38	ETL. Deposition. Procedure [Proc. 1 >> Proc. 2 >> ... | Proc. 3 >> ... | Proc	Spray-pyrolys | Spin-coating >> Spin-coating
39	ETL. Deposition. Aggregation state of reactants (Liquid/Gas/Solid) [Agr.	Liquid | Liquid
40	ETL. Deposition. Synthesis atmosphere [Gas1; Gas2 >> Gas3; ... >> ... | G	Air; O2 | Air
41	ETL. Deposition. Synthesis atmosphere. Pressure. Total [P.1 >> P.2 >> ...	1 atm | 1 atm
42	ETL. Deposition. Synthesis atmosphere. Pressure. Partial [P.1; P.2 >> P.3	1 atm; 1 bar | 1 atm
43	ETL. Deposition. Synthesis atmosphere. Relative humidity [RH1 >> RH2 >	35 | 35
44	ETL. Deposition. Solvents [Sol.1; Sol.2 >> Sol.3; ... >> ... | Sol.4 >> ... | So	Acetonitil; Acetyl aceton; IPA | Ethanol >> Acetonitrile
45	ETL. Deposition. Solvents. Mixing ratios [V1; V2 >> V3; V4 >> ... | V5; V6	9:0.4:0.6 | 1 >> 1
46	ETL. Deposition. Solvents. Supplier [Sup.1; Sup.2 >> Sup.3; ... >> ... | Sup	Sigma Aldrich; Sigma Aldrich; Fisher | Sigma Aldrich >> Acros
47	ETL. Deposition. Solvents. Purity [Pur.1; Pur.2 >> Pur.3; ... >> ... | Pur.4 >	Pro analysis; Pro analysis; Pro analysis | Puris >> Pro analysis
48	ETL. Deposition. Reaction solutions. Compounds [C1; C2 >> C3; ... >> ... | C	Titanium diisopropoxide bis(acetylacetonate) | TiO2-np >> Li-TFSI
49	ETL. Deposition. Reaction solutions. Compounds. Supplier [Sup.1; Sup.2 >	Sigma Aldrich | Dysole >> Sigma Aldrich
50	ETL. Deposition. Reaction solutions. Compounds. Purity [Pur.1; Pur.2 >> P	Pro analysis | Tecnical >> Pro analysis
51	ETL. Deposition. Reaction solutions. Concentrations [c1 M; c2 mol/dm3 >>	6 vol% | 150 mg/ml >> 10 mg/ml
52	ETL. Deposition. Reaction solutions. Volumes [V1 >> V2 >> ... | V3 >> ...	10 | 0.05 >> 0.05
53	ETL. Deposition. Reaction solutions. Age [A1 >> A2 >> ... | A3 >> ... | A4	0.5 | 1000 >> 1000

More ”comfortable” data entry

The Perovskite database

”GUI or electronic lab notebook”

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Bibliographic | Device | Compounds | Cell | Module | Analysis | KPIs

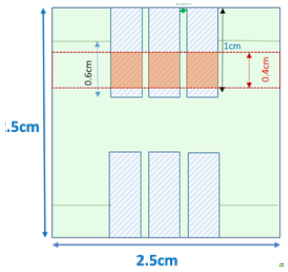
Device layout

Substrate area [ ] [ ] (unit)

# of pixels [ ]

Test cell area [ ] [ ] (unit)

Schematic Device Layout



Further Information

Free text

Device Layer stack

pin [X]
nip [ ]

Schematic

Substrate
HTM
Perovskite
ETL
Back contact
⊕ Add layer

Single Layer Definition: Perovskite Absorber

Solution processed [X]
Vapor deposition [ ]

Precursor Ink | Dep. Method | Analysis | KPIs

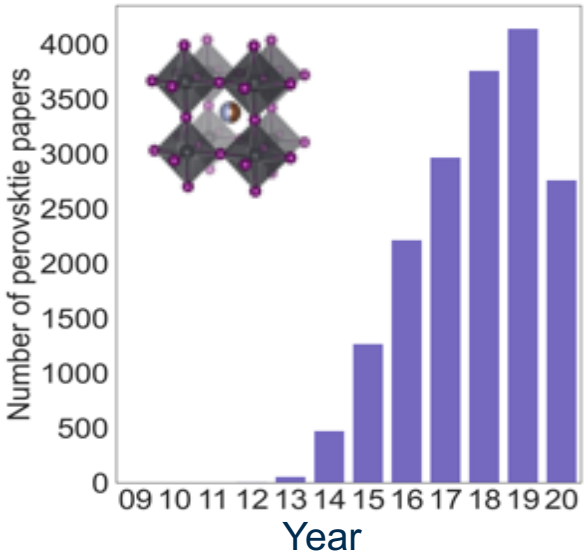
Precursor(s) [ ] [ ] (unit)

Additive(s) [ ] [ ] (unit)

Solvent(s) [ ] [ ] (unit)

Link to ”chemical database”/compounds

Step 2: Recruiting volunteers to help us



16 000 / 80
= 200 papers each

”Perovskite Solar Cells”*:
> 16 000 papers published

Step 3: Launch database

www.perovskitedatabase.com

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Interactive graphics

To facilitate easy exploration of the perovskite data we have developed a set of interactive graphics tools. Those enable simple interactive exploration of the data in the database. The interactive graphics are hosted by Materials Zone. To reach the graphics you will need to create a free account. To access the interactive graphics, you will need to fill out this form. Shortly after filling out the form, you will receive an invitation by email.

Figures generated by the interactive graphics are free to be used in any way.

Fill out the form to access the interactive graphics

There are now 9 apps focusing on different aspects, with more to come.

Figures generated by the interactive graphics are free to be used in any way.

The apps are found under “Insights >> Perovskite Database Project” in the left side menu in Materials Zone’s system found on the link below (see instructions above on how to obtain access to the interactive graphics)

Link to interactive graphics

General development

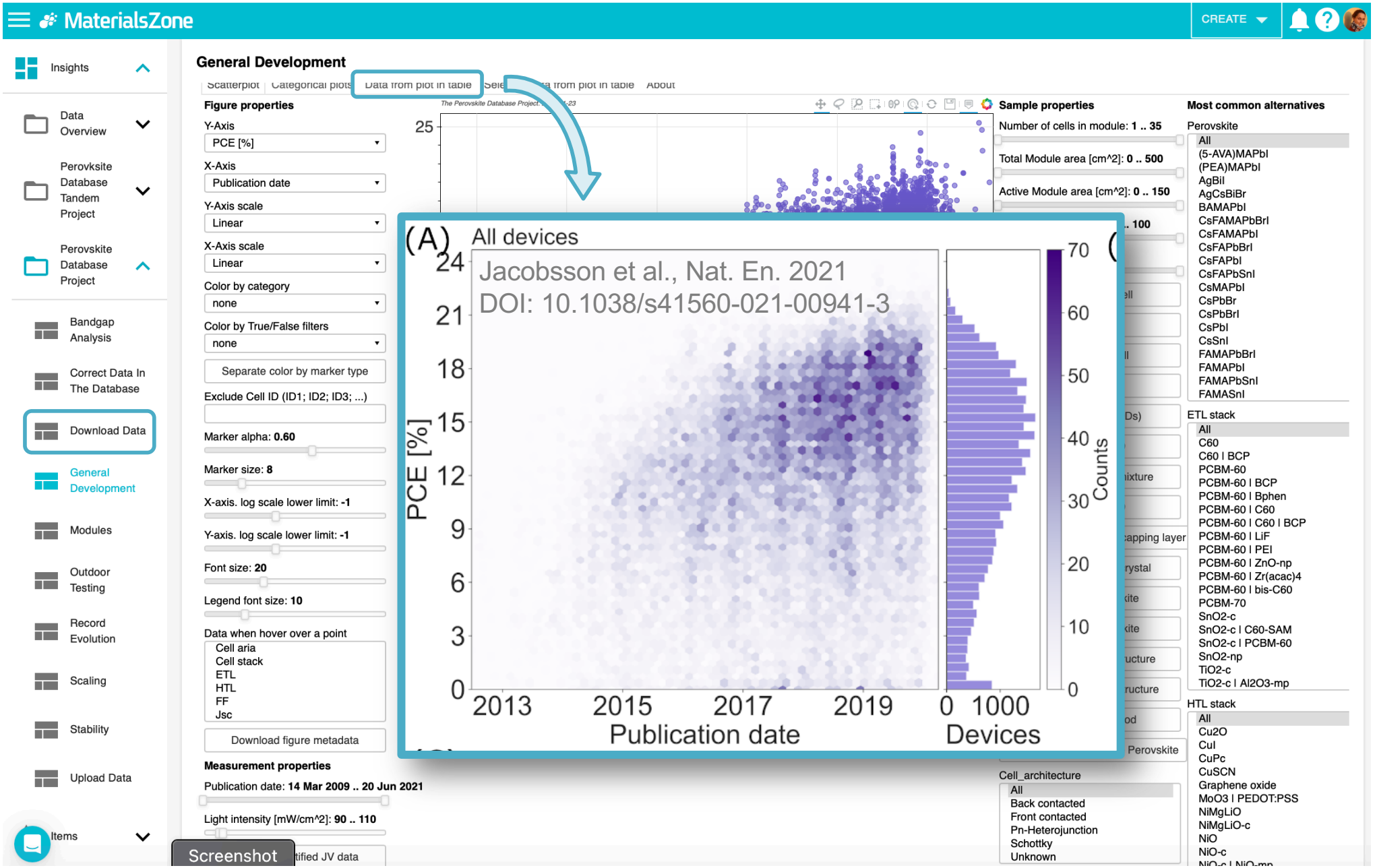
Focuses on the development of general device performance and enables filtering within the entire dataset

Example: Evolution of reported PCEs as function of publication date

You can download generated plots as figures and re-use.

The Perovskite Database: A secondary dissemination platform

www.perovskitedatabase.com: You can download the data and replot however you like to re-use.

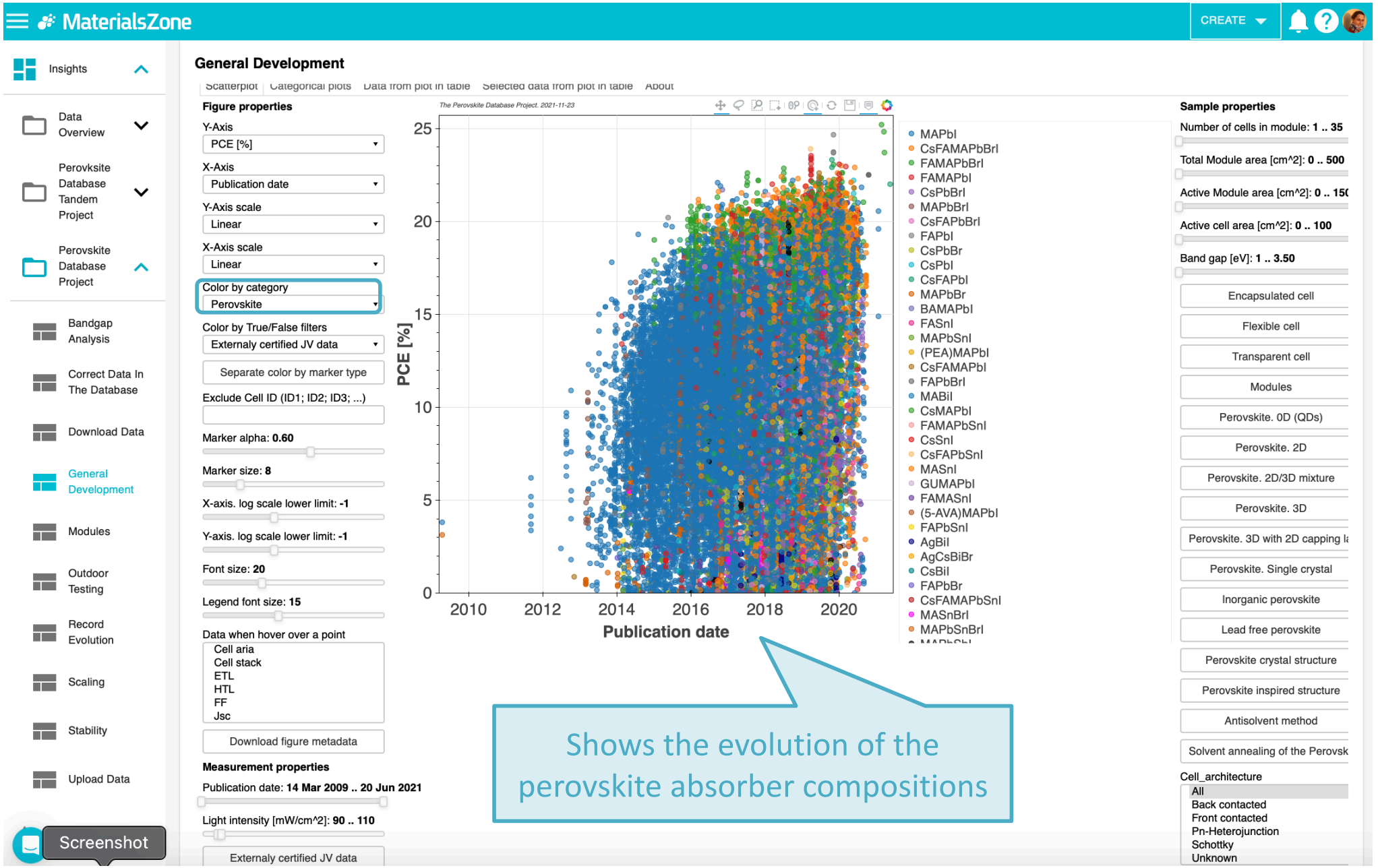


Example: Evolution of reported PCEs as function of publication date

You can emphasize datapoints in the dataplots (example: certified data)

Example: Evolution of reported PCEs as function of publication date

You can highlight different data categories to view trends (example: perovskite composition)



Example: Evolution of reported PCEs as function of publication date

Pick data-sets you find most interesting (example: evolution of perovskite compositions)

Jacobsson et al., Nat. En. 2021
DOI: 10.1038/s41560-021-00941-3

Outlook…

You note that collected data thins-out after 2020…

Strategies to keep feeding the database

Join: sign up via www.perovskitedatabase.com

Use the data available for anything you want

You can download plots as well as the complete dataset: use it!

Make YOUR resarch data easier to find

Upload all your experimental perovskite PV datasets to The Perovskite Database upon publication and link to DOI of your article (fullfills ”OpenScience” requirements!)

Upload other’s work & spread the word

Invite and make others aware of the project

Check data that is online for inconsistencies

Remove/correct with correct data function

Become involved feeding the database

We hope this to become a community-driven project

VIPERLAB

If you want to start a specific expansion of the database, please submit proposal via VIPERLAB.

Remaining OPEN: Initiation of collaborative review papers

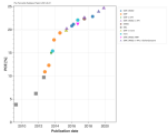
List of ongoing collaborative research papers available on www.perovskitedatabase.com

My Drafts 4 Public Documents 0

June 01, 2021

Insights from the Perovskite Database Project: Ink formulation evolution

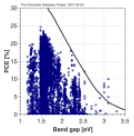
eva.unger, oleksandra.shargaieva, jinzhao.li, et al.



May 25, 2021

"Collective Insight from the Perovskite Database Project": Bandgap Tuning of Metal-Ha...

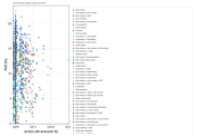
eva.unger, oleksandra.shargaieva, klara.suchan, et al.



June 01, 2021

Insights from the Perovskite Database Project: Scalable Manufacturing Methods

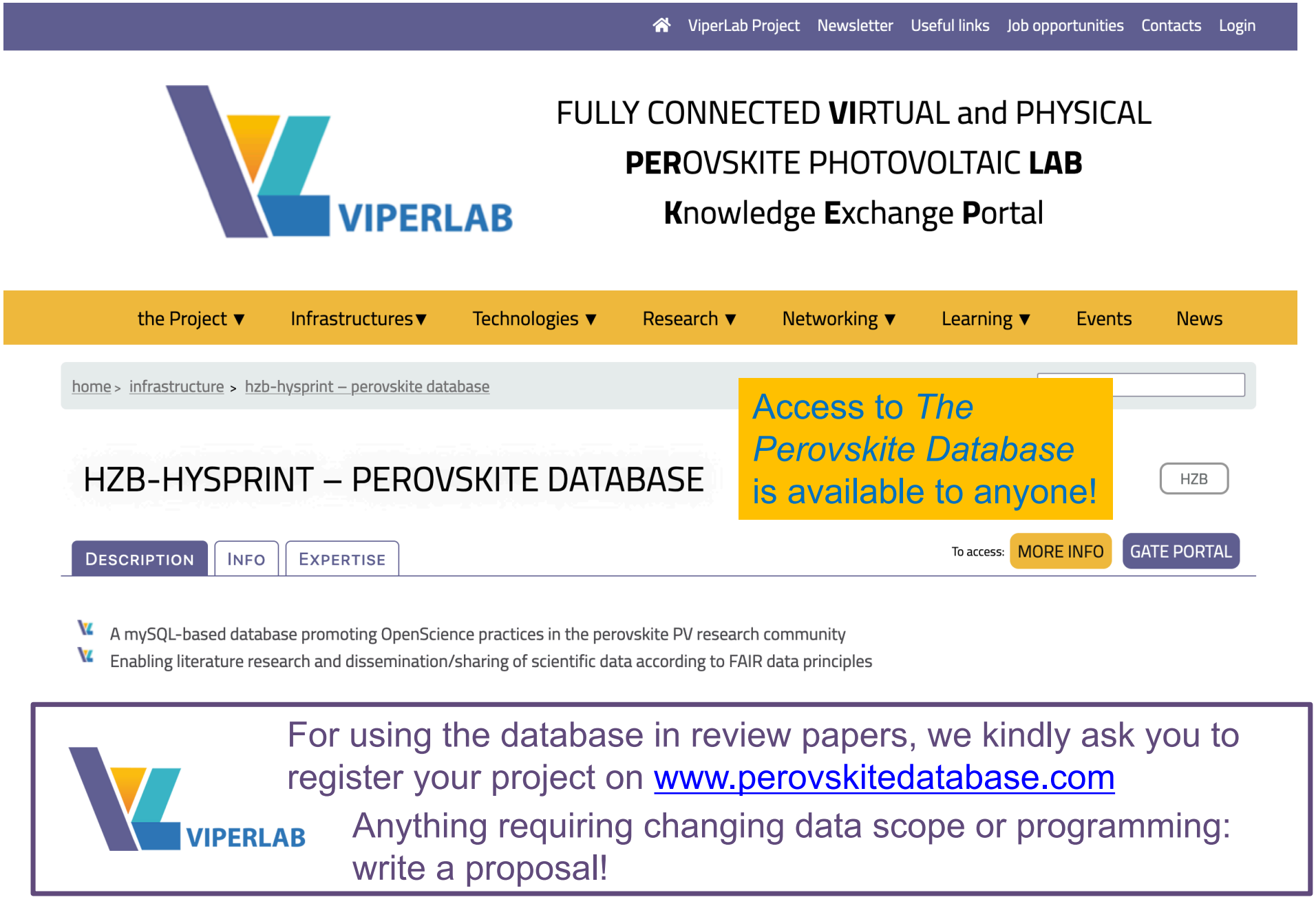
eva.unger, gopinath.paramasivam, jinzhao.li, et al.



VIPERLAB

You have an idea for a review paper based on the data available?
Write short proposal to be submitted via VIPERLAB Gate
(or write me a brief e-mail: eva.unger@helmholtz-berlin.de)

The Perovskite Database Expansion in VIPERLAB

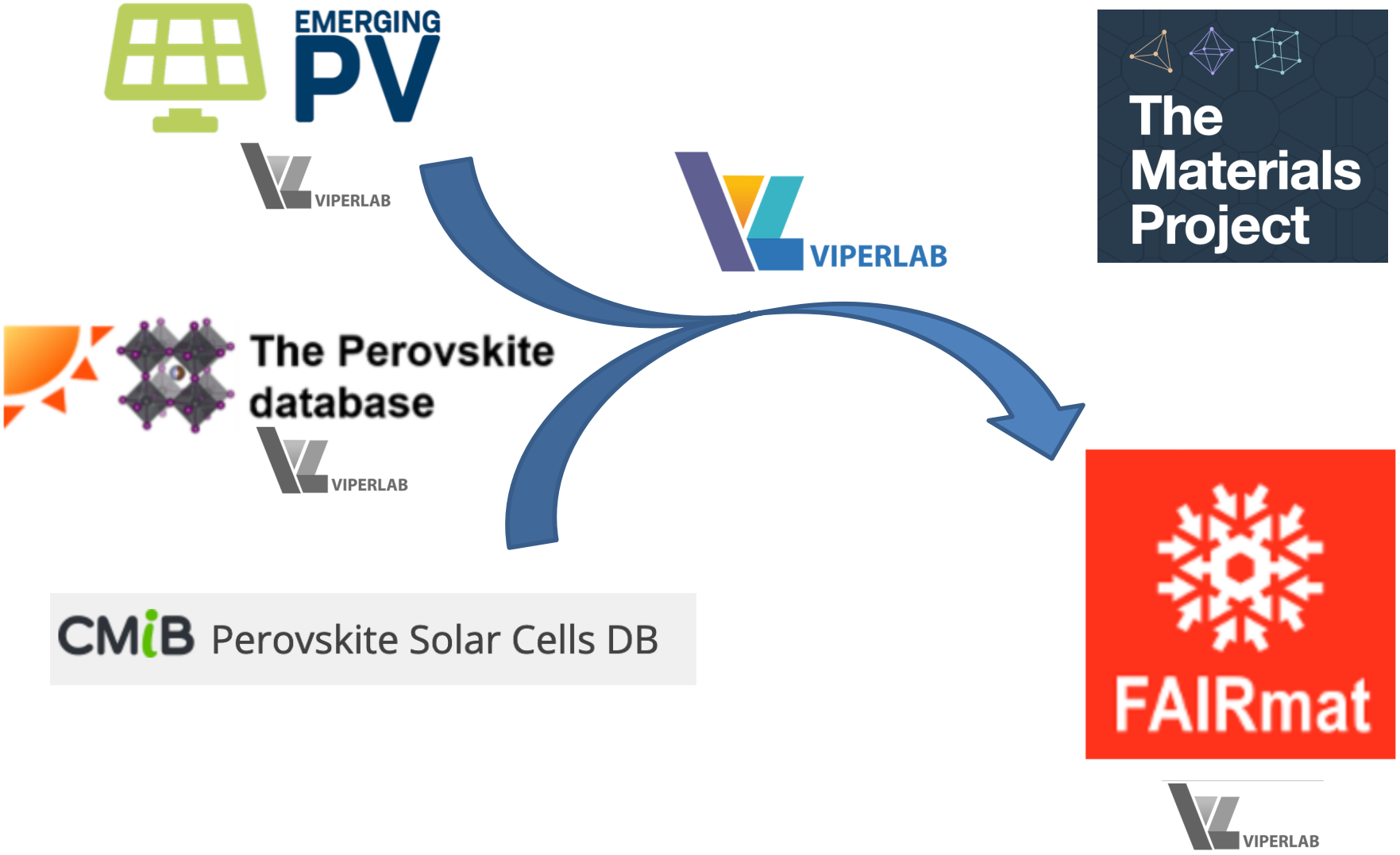


VIPERLAB

For using the database in review papers, we kindly ask you to register your project on www.perovskitedatabase.com

Anything requiring changing data scope or programming: write a proposal!

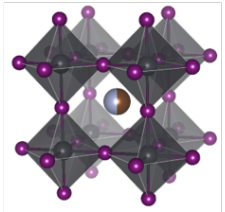
Related Relevant Data Infrastructures



Acknowledgement

Dr. Jesper Jacobsson (tenure track Professor @ Nankai University in China)

The Perovskite Database



GRECO

www.greco-project.eu

VIPERLAB

www.viperlab.eu

Please all join! Just sign up!

www.perovskitedatabase.com

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eva.unger@helmholtz-berlin.de