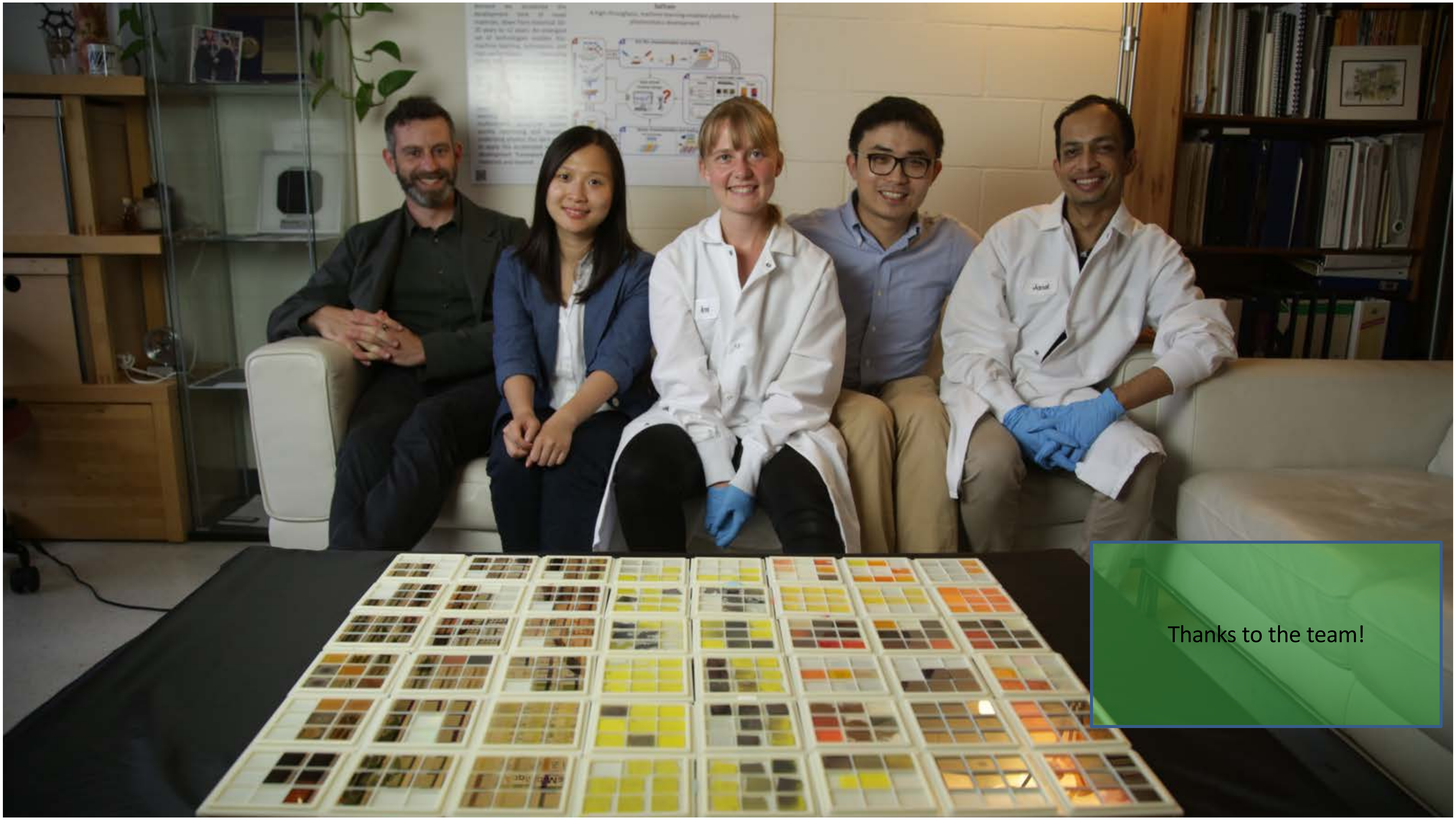
Inverse Design: Why Aren't We There Yet?

Tonio Buonassisi (MechE, MIT)

Accelerated Materials Laboratory for **Sustainability**

General Inverse Design of Crystalline Materials:
Why Aren't We There Yet?

A refinement of the broader title. This presentation focuses on crystalline inorganic materials.



Thanks to the team!

Thanks to the team!

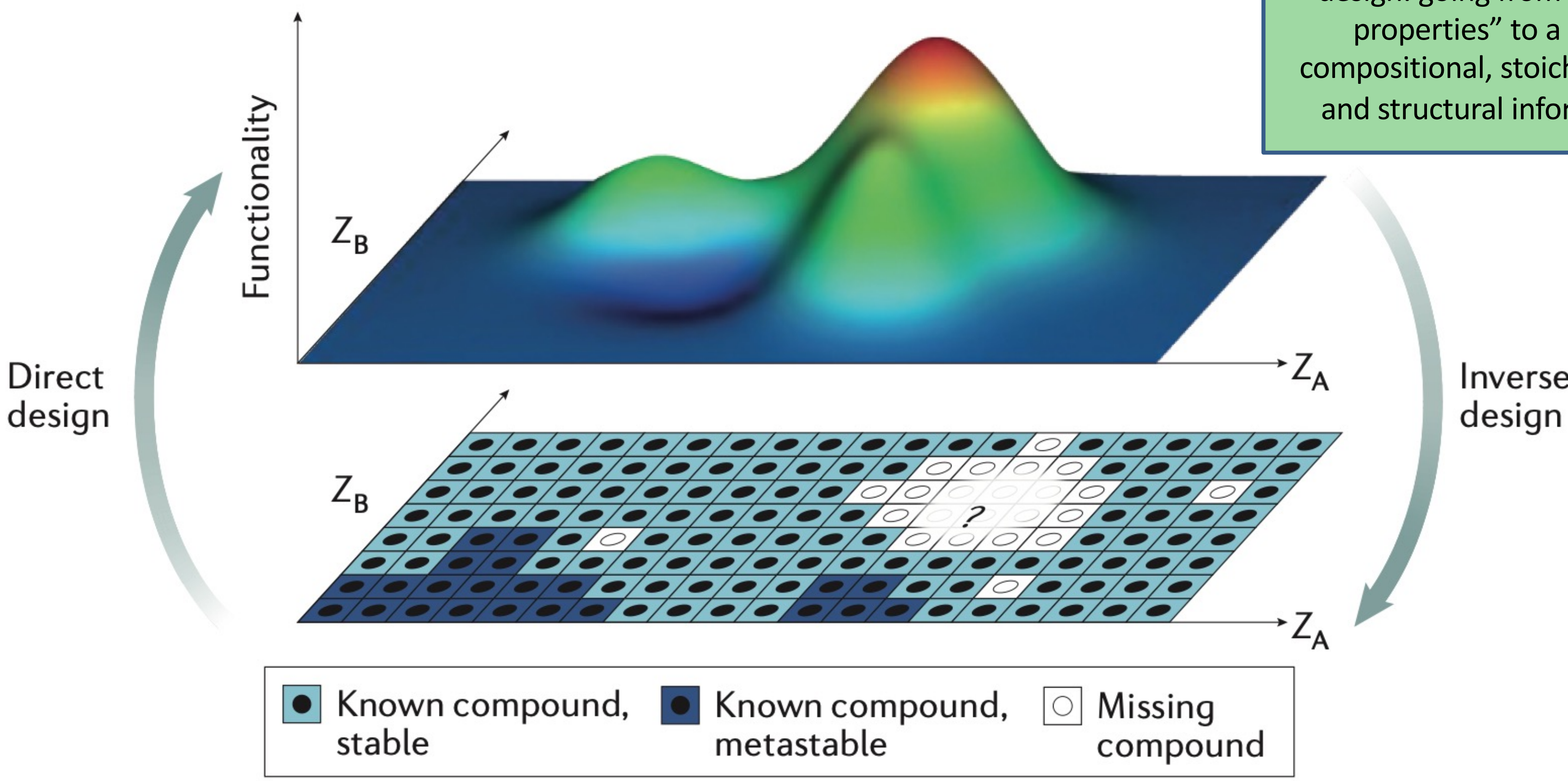
Goal:

You give me a set of properties,
I give you a material.

This is the goal of inverse design

Materials Prediction from Property Sets

Alex Zunger's framing of inverse design: going from "desired properties" to a set of compositional, stoichiometric, and structural information.



A. Zunger, *Nat. Rev. Chem.* **2**, 121 (2018)
https://doi.org/10.1038/s41570-018-0121

History: US-Based Research Centers

Center for Inverse Design
Achieving the grand challenge of materials and nanostructures by design

CNGMD
Incorporating Metastability

These EFRCs (Energy Frontier Research Centers), led out of Colorado, focused heavily on inverse design. The latter, included the Materials Project team and the presenter.

PERSPECTIVES

Inverse design in search of materials with target functionalities

Alex Zunger

Abstract | Solid-state chemists have been consistently successful in envisioning and making new compounds, often enlisting the tools of theoretical solid-state physics to explain some of the observed properties of the new materials. Here, a new style of collaboration between theory and experiment is discussed, whereby the desired functionality of the new material is declared first and theoretical

Because properties live in certain ACSs and not in others, the fundamental question in solid-state chemistry, condensed-matter physics, metallurgy and organic matter is: can we uncover the 'genetic code' of structure–property (or body–soul) relations?

The properties required to realize a particular device are often known, but the specific materials that harbour such properties are generally unknown and are difficult to identify. The conditions needed for water splitting, the defining qualities of coexisting transparency and conductivity in transparent conductors, and the reason

A. Zunger, *Nat. Rev. Chem.* **2**, 121 (2018)
https://doi.org/10.1038/s41570-018-0121

PERSPECTIVES

Challenge #1: “Technological applications often demand compounds with what would appear to be a counterintuitive combination of two or more properties. Such compounds harbouring what appears as contradicting attributes are rather difficult to identify and discover.”

Invers… with t…

Alex Zunger

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PERSPECTIVES

Challenge #2: "Because the effective interactions used as input are generally not expressible (or mappable) in terms of the periodic table, there is generally no recognizable rational path between model Hamiltonian predictions and the realization of actual materials. In other words, the theory is not invertible."

Invers
with t

Alex Zunger

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PERSPECTIVES

Invers
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Alex Zunger

Challenge #3: "because the total electron and ion energy of the system is generally not computed or optimized with respect to the structural degrees of freedom, it is difficult to assess whether the predicted properties (such as exotic superconductivity and quantum spin liquids) will be found in stable (or nearly stable) recognizable compounds"

Abstract | Solid-state chemists have been consistently successful in envisioning and making new compounds, often enlisting the tools of theoretical solid-state physics to explain some of the observed properties of the new materials. Here, a new style of collaboration between theory and experiment is discussed, whereby the desired functionality of the new material is declared first and theoretical

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A. Zunger, *Nat. Rev. Chem.* **2**, 121 (2018)
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Generative Design & Inverse Design

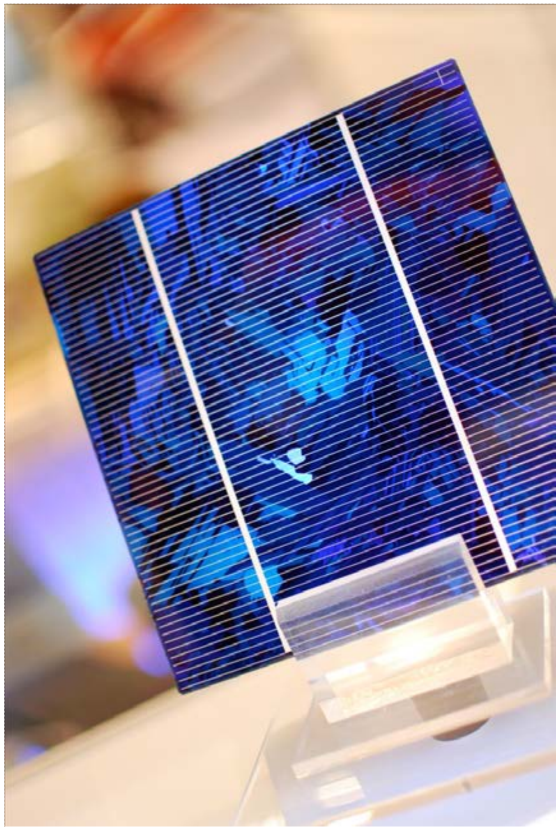
As our community struggles for common definitions, here are my definitions of these two terms with examples.

Generative Design

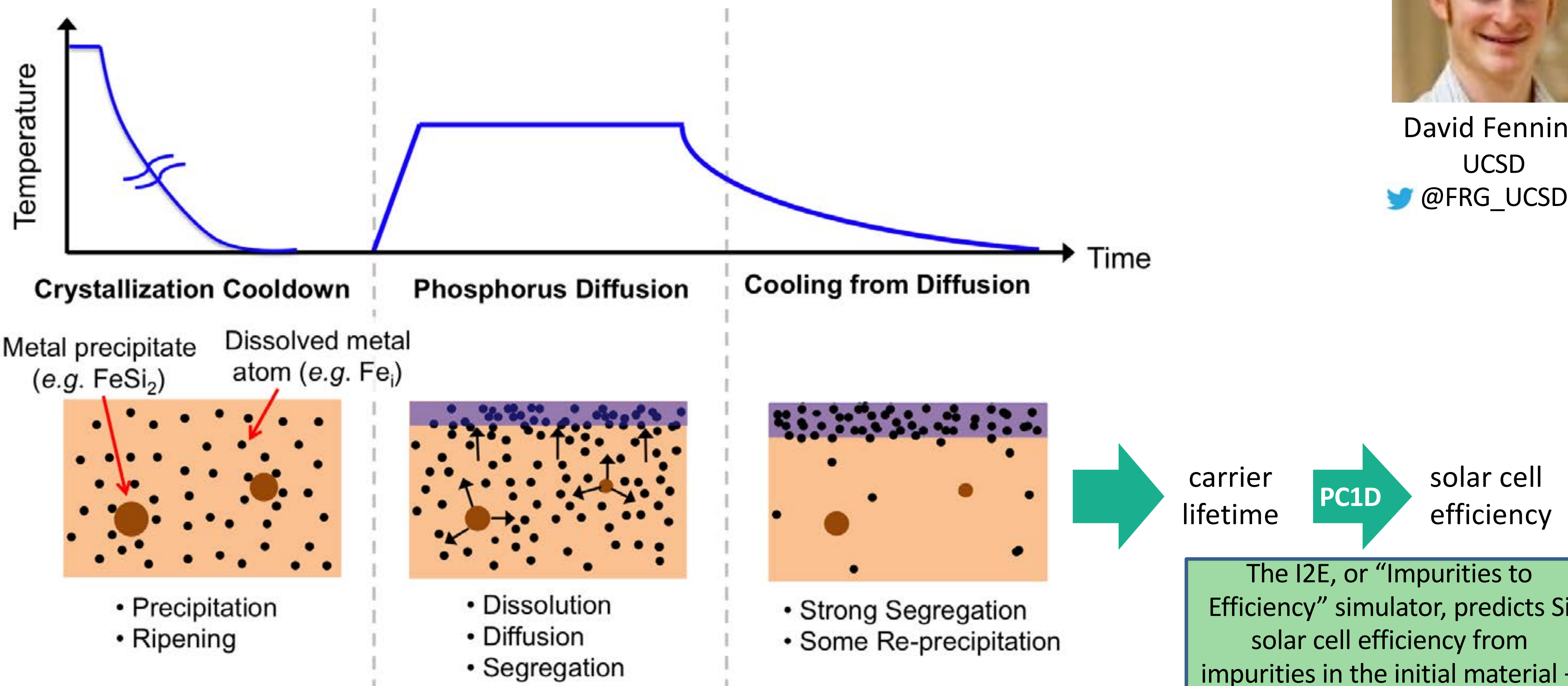
"Generative design is an iterative design process that involves a program that will generate a certain number of outputs that meet certain constraints, and a designer that will fine tune the feasible region by selecting specific output or changing input values, ranges and distribution."

https://en.wikipedia.org/wiki/Generative_design

2014: Generative Design in Silicon Solar Cell Manufacturing



2014: Generative Design in Silicon Solar Cell Manufacturing

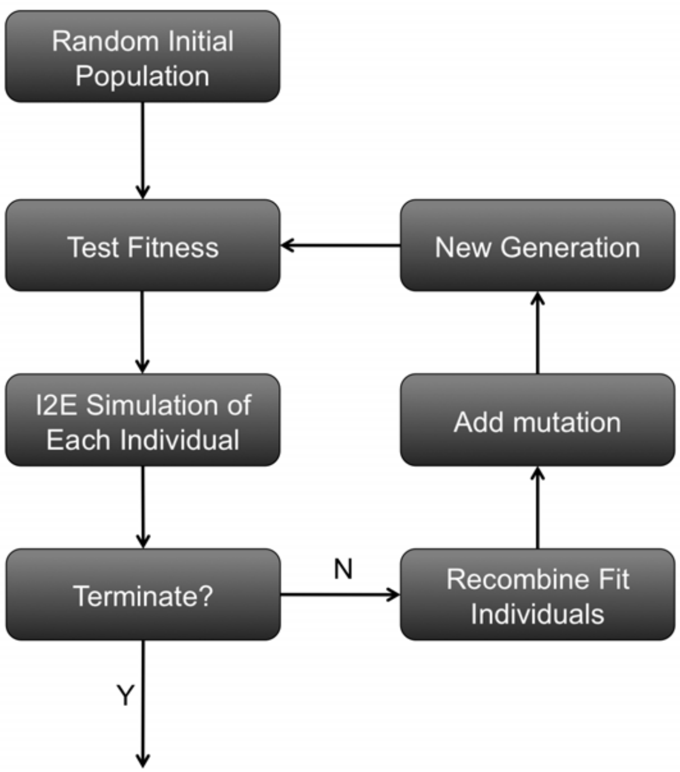


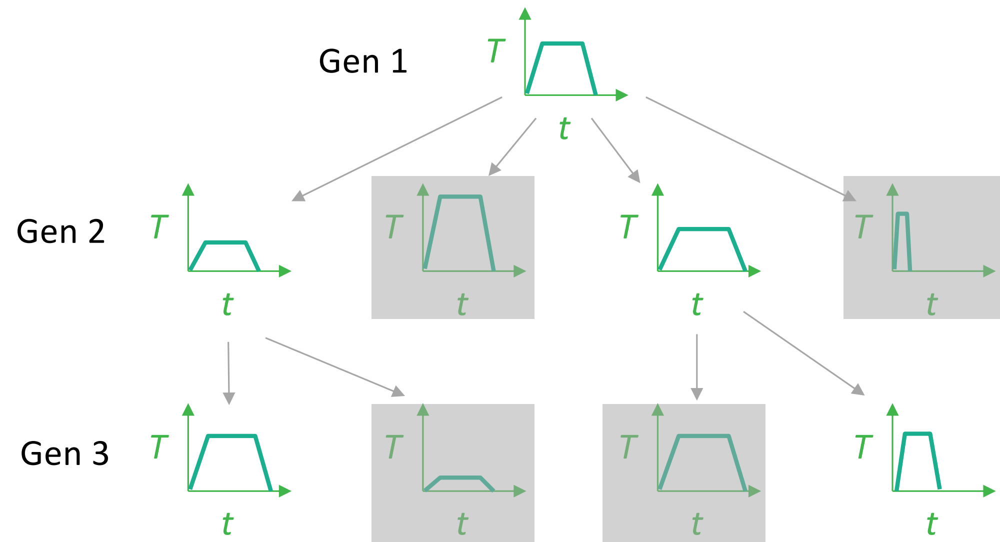
David Fenning
UCSD
@FRG_UCSD

The I2E, or "Impurities to Efficiency" simulator, predicts Si solar cell efficiency from impurities in the initial material + process conditions

D.P. Fenning *et al*., *Adv. Energy Mater*. 1400459 (2014)
https://doi.org/10.1002/aenm.201400459

2014: Generative Design in Silicon Solar Cell Manufacturing





The I2E tool can be wrapped in a Genetic Algorithm, creating new time-temperature profiles from an original time-temperature profile.

D.P. Fenning *et al.*, *Adv. Energy Mater*. 1400459 (2014)
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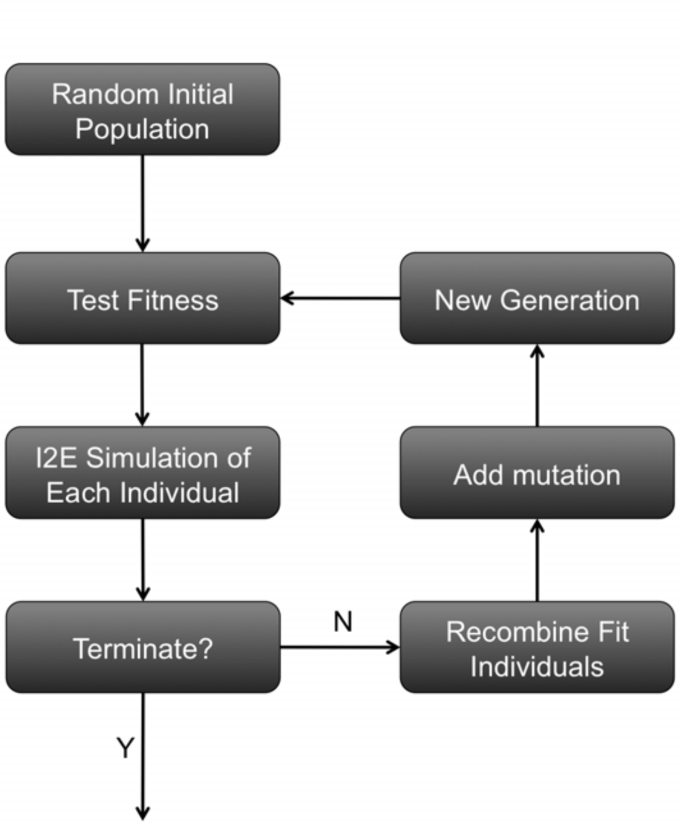
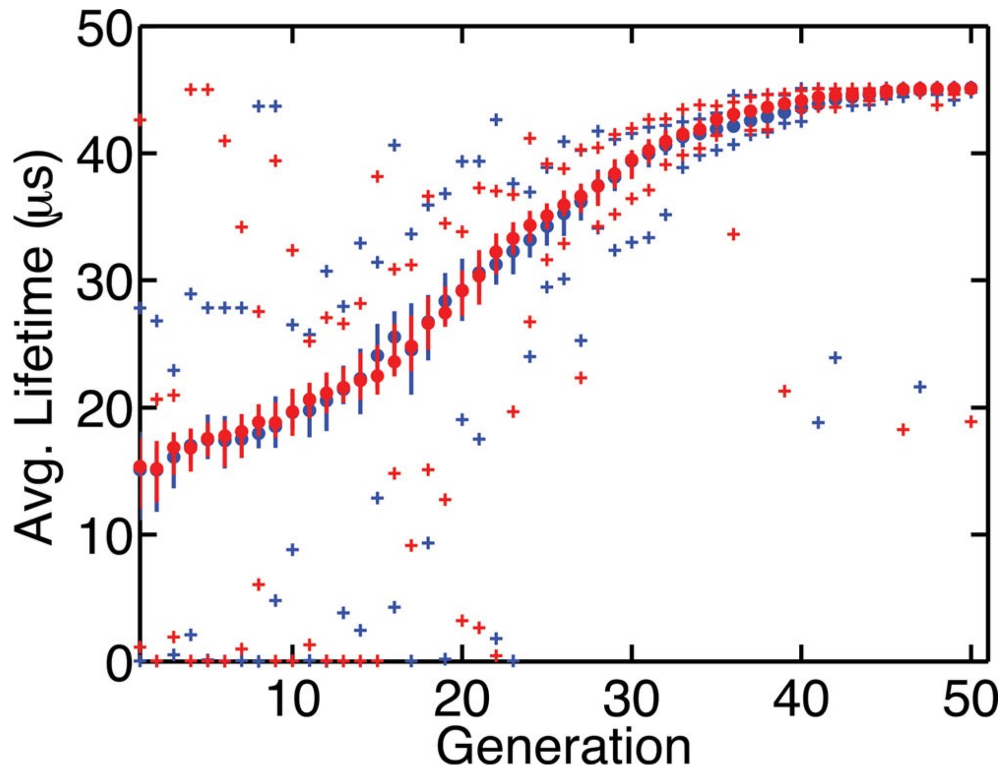
2014: Generative Design in Silicon Solar Cell Manufacturing





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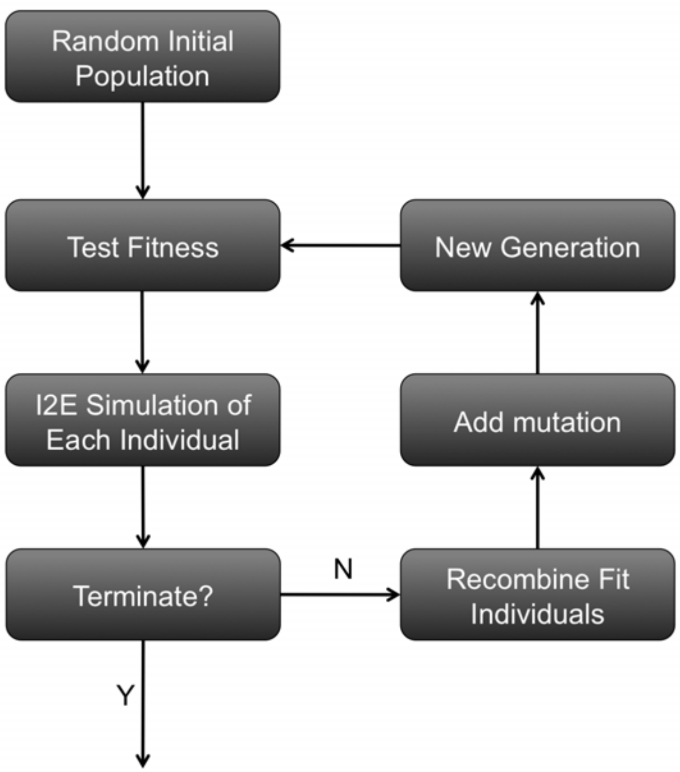

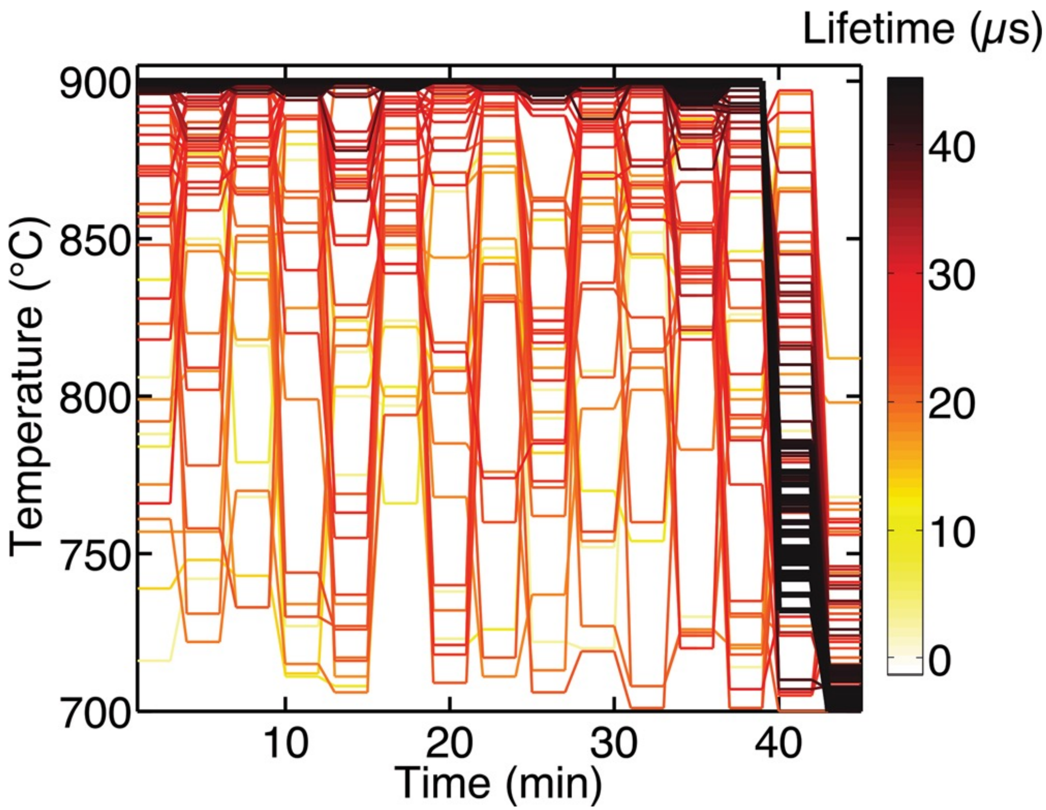

D.P. Fenning *et al.*, *Adv. Energy Mater*. 1400459 (2014)
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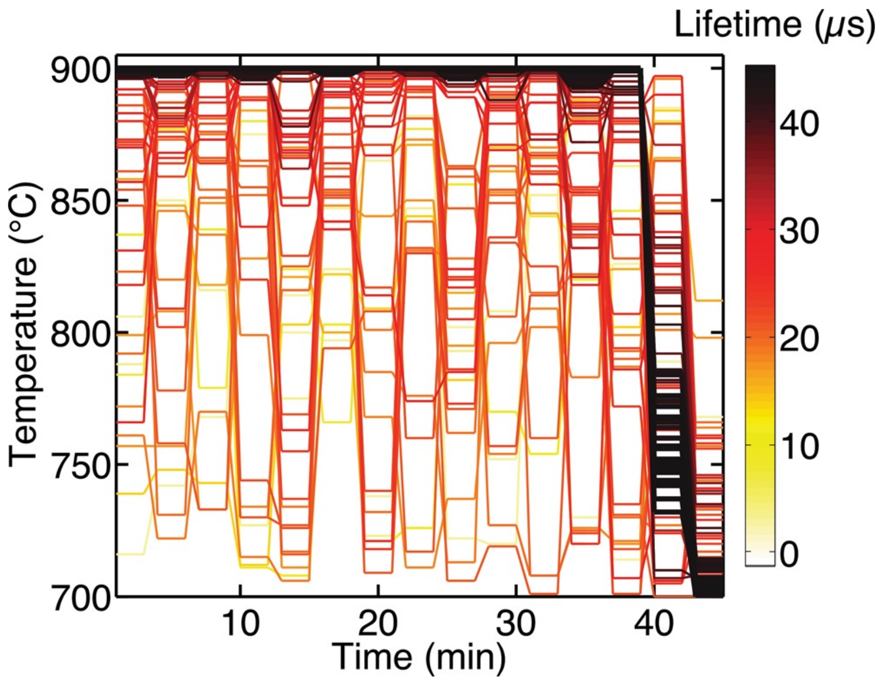
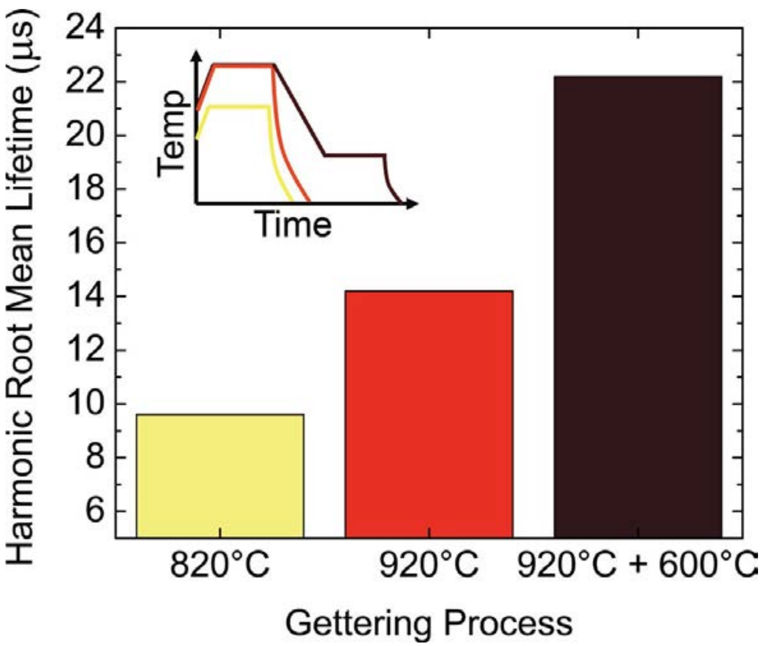
2014: Generative Design in Silicon Solar Cell Manufacturing

Prediction



Experiment



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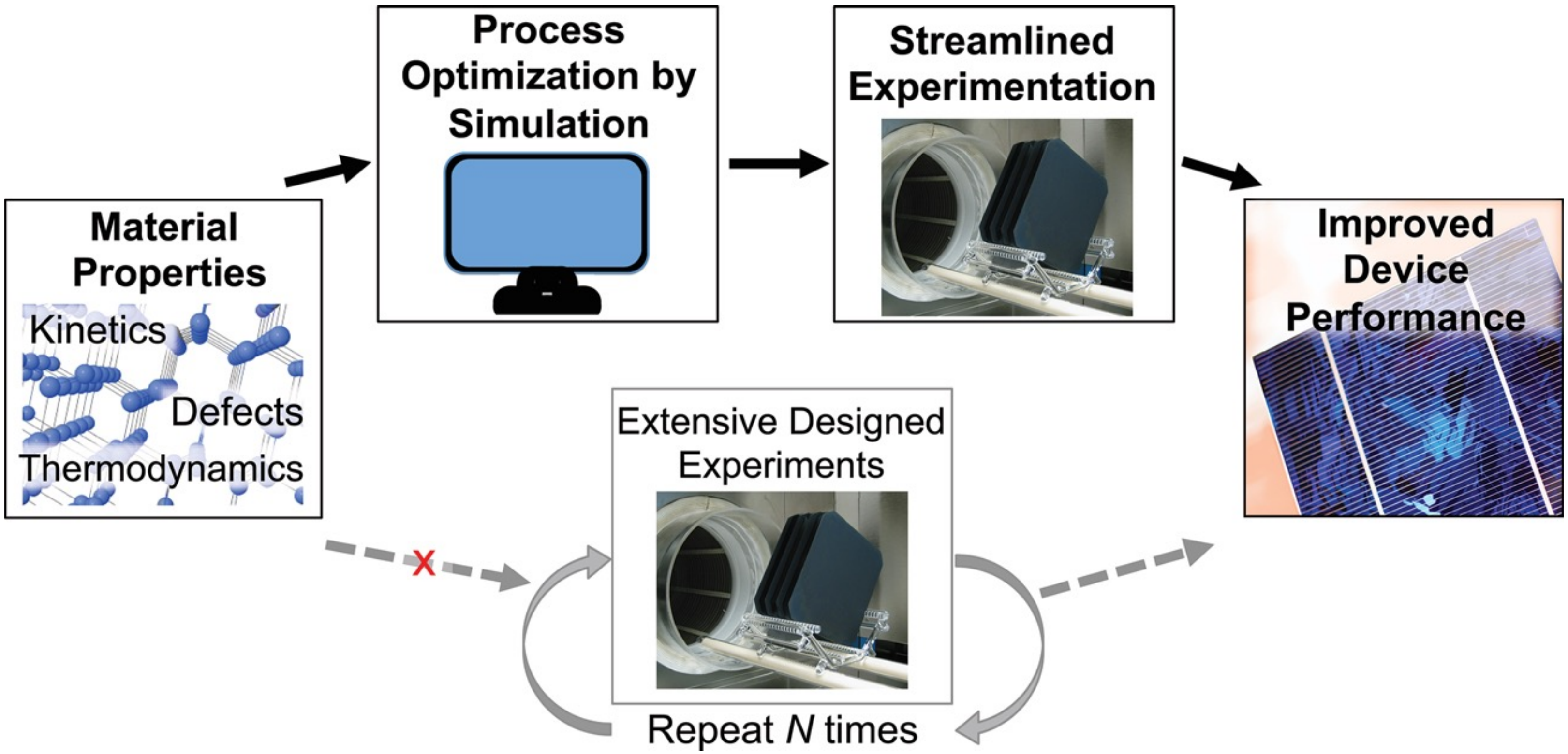

D.P. Fenning *et al*., *Adv. Energy Mater*. 1400459 (2014)
https://doi.org/10.1002/aenm.201400459 Buonassisi — MIT — 20220815

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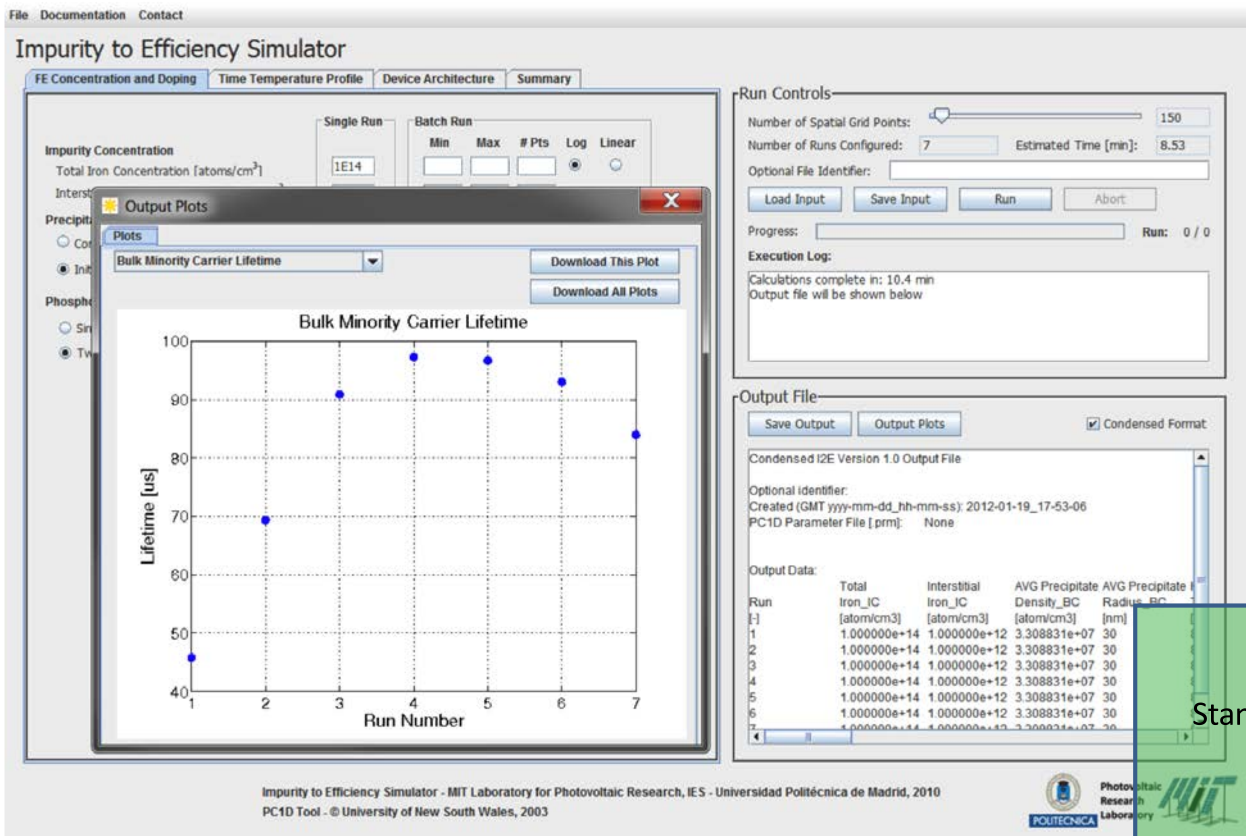
2014: Generative Design in Silicon Solar Cell Manufacturing

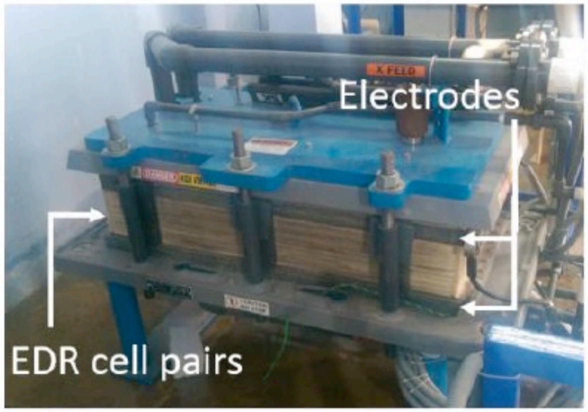


Stand-alone GUI for the I2E simulator

D.P. Fenning *et al.*, *Adv. Energy Mater*. 1400459 (2014)
https://doi.org/10.1002/aenm.201400459

2017: Solar-Powered Desalination System Optimization

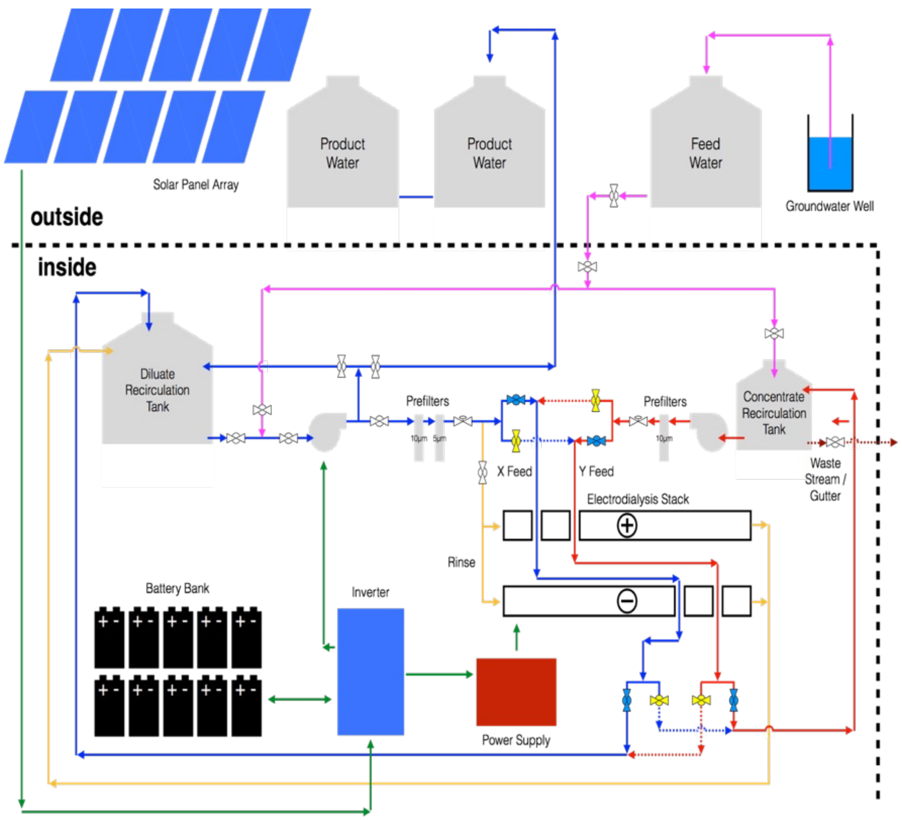
Sterling Watson
MIT; Natel Energy

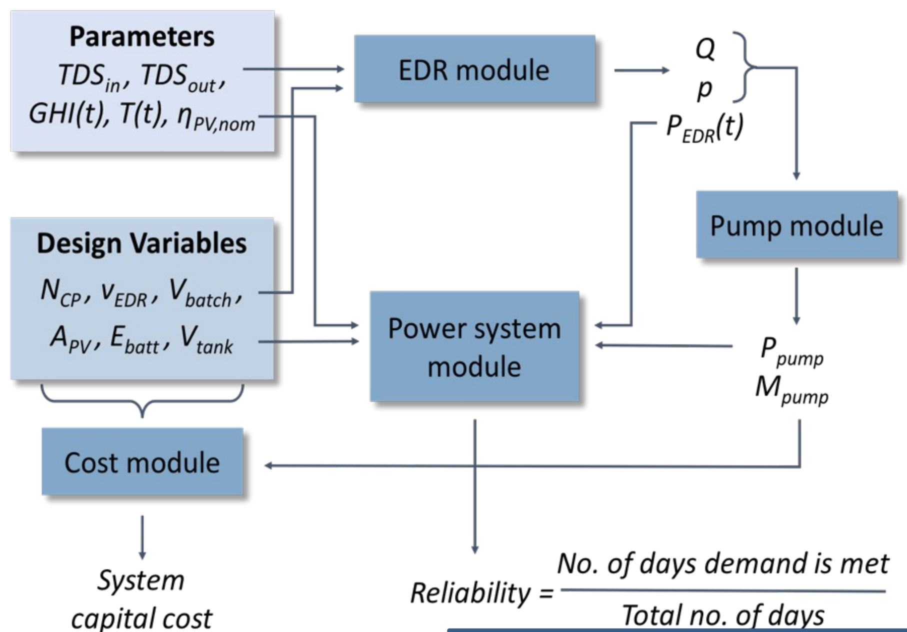


Another example of generative design in sustainability, a collaboration with the GEAR Lab at MIT (Amos Winter)

S. Watson *et al.*, *Solar Energy* **162**, 132–139 (2018)
https://doi.org/10.1016/j.desal.2019.114217

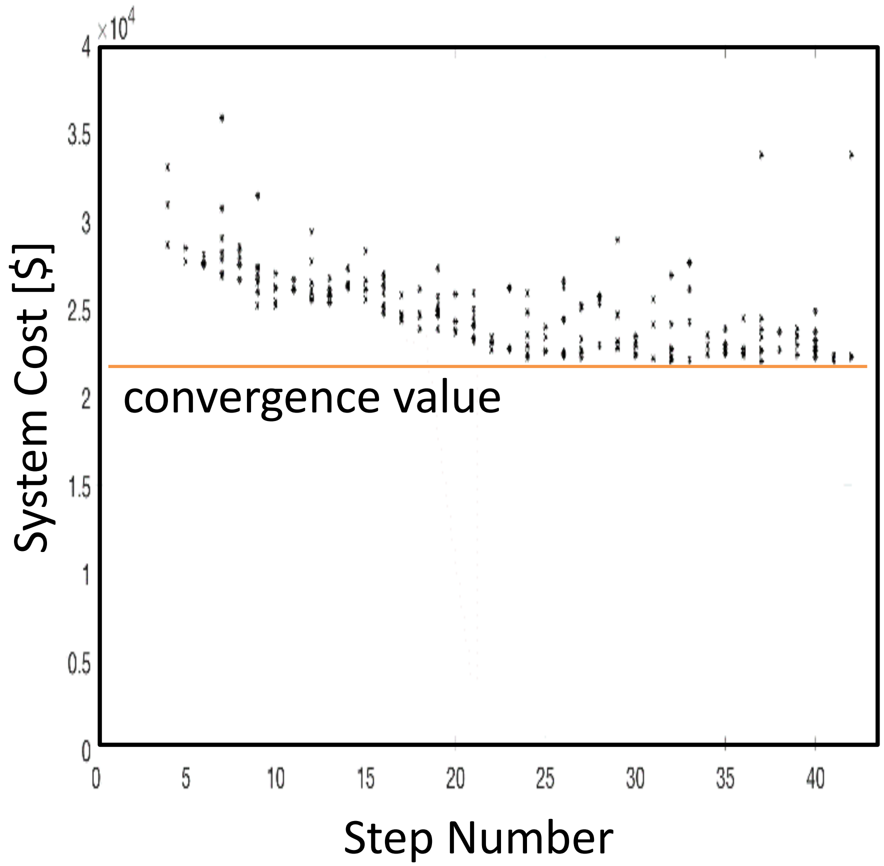
2017: Solar-Powered Desalination System Optimization

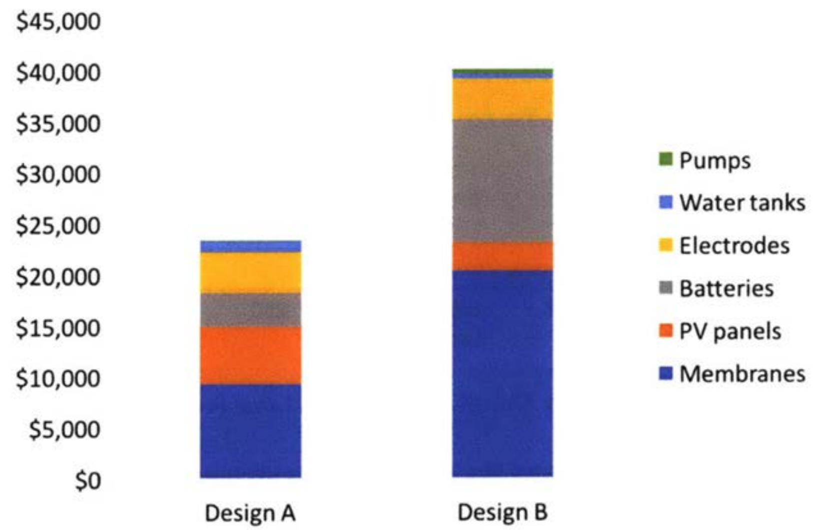




Again, system of equations is well defined, and a forward model can be created.

2017: Solar-Powered Desalination System Optimization





A nearly 40% drop in system cost can be achieved through particle swarm optimization, with this forward model.

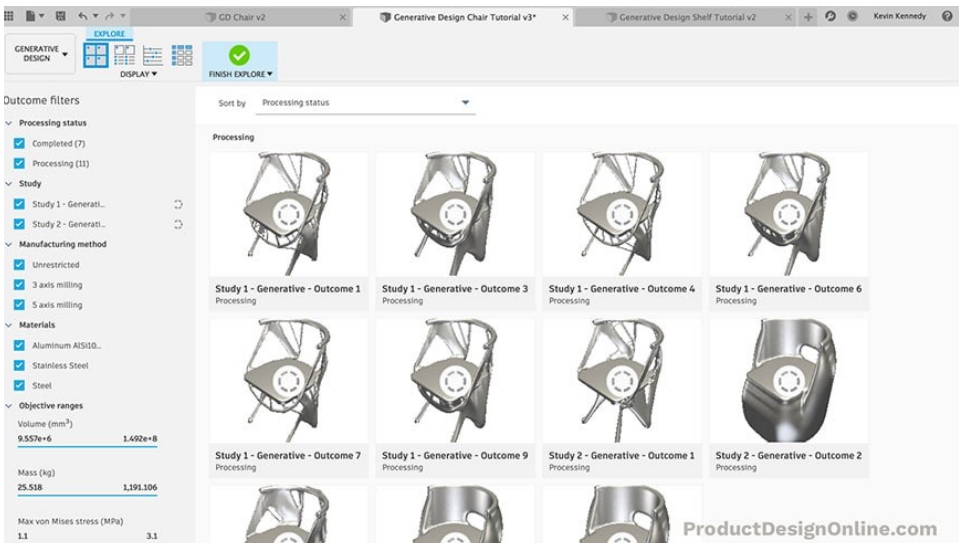
S. Watson *et al.*, *Solar Energy* **162**, 132–139 (2018)
https://doi.org/10.1016/j.desal.2019.114217

2017: Solar-Powered Desalination System Optimization

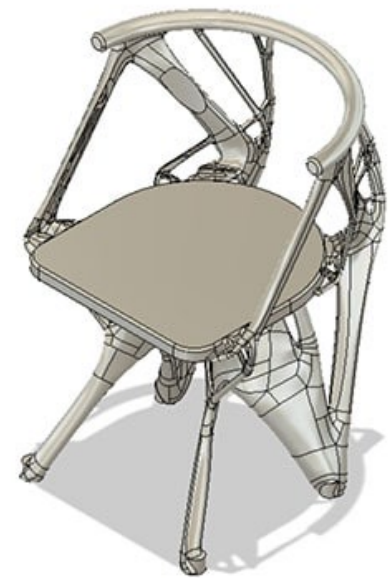
Designed and built a cost-optimized PV-EDR system in Chellur, India

S. Watson *et al.*, *Solar Energy* **162**, 132–139 (2018)
https://doi.org/10.1016/j.desal.2019.114217

AutoCAD - Fusion 360: Constrained Generative Design



https://productdesignonline.com/fusion-360-tutorials/generative-design-a-stronger-chair-in-fusion-360/



A commercial example

Generative Design Approach

define target properties

define input variables

run simulation

calculate output parameter(s) of merit

iterate until target reached

This is how we did it so far… embed a simulation (forward model), iterate inputs until converged on user-defined target properties.

Generative Design Approach

define target properties

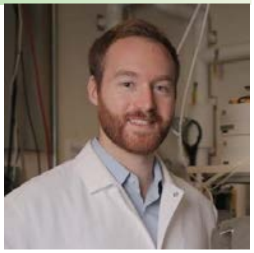
define input variables

search database

identify materials
with target properties

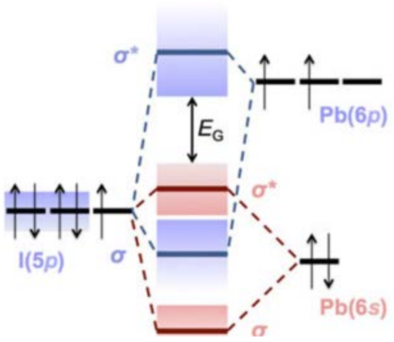
With Materials Project and other open-source databases, we could now search those databases for materials with user-defined properties.

2015: Screening Materials Project with "Transport" Proxies

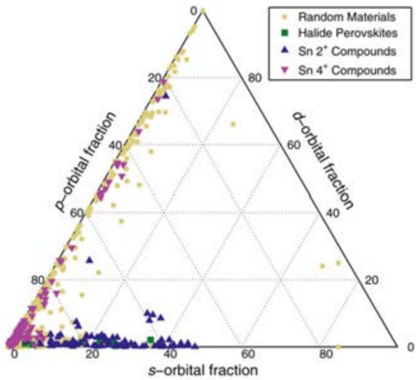


Riley Brandt

Determine Params of Merit



Screen Params of Merit



R.E. Brandt *et al.*, *MRS Communications* **5**, 265 (2015)
http://dx.doi.org/10.1557/mrc.2015.26

2015: Screening Materials Project with "Transport" Proxies

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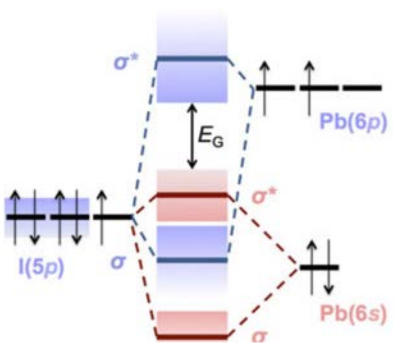
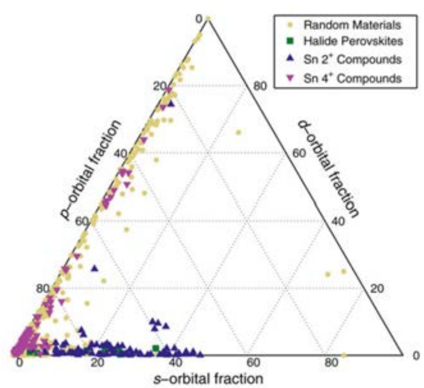


Screen Params of Merit



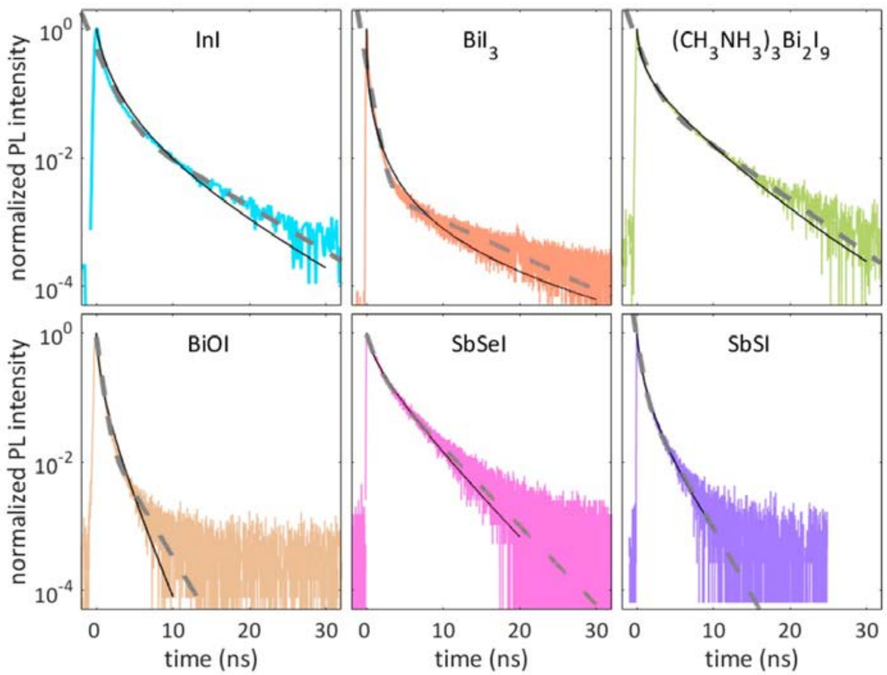
MRS Communications

Table I. DFT-computed band structures, band dispersion (with SO coupling), effective masses, and ionic dielectric constants for several compounds of interest, as compared with the (MA)BX_3 family of perovskites.

Formula	Space Group (International S. G. number)	E_G (eV) (DFT+SO)	E_G direct (eV) (DFT + SO)	E_G (DFT + SO)— E_G (DFT)	E_V (DFT + SO)— E_V (DFT)	E_C (DFT + SO)— E_C (DFT)	m_h^* (DOS)	m_e^* (DOS)	VBM band degeneracy	CBM band degeneracy	Ionic dielectric constant
InI	*Cmcm* (63)	1.29	1.29	−0.09	0.08	−0.01	0.25	0.15	2	2	33.51
SnI_2	*C12/m1* (12)	1.58	1.74	−0.18	0.10	−0.08	1.49	0.35	4	2	28.84
SbI_3	$R\bar{3}H$ (148)	1.88	1.96	−0.26	0.18	−0.08	9.57	2.12	1	1	8.32
SbI_3	$P12_1/c1$ (14)	1.86	1.93	−0.25	0.18	−0.07	8.88	1.72	2	1	8.43
BiI_3	$R\bar{3}H$ (148)	1.73	1.82	−0.78	0.23	−0.55	10.39	1.85	1	1	5.70
BiI_3	$P\bar{3}\,1m$ (162)	1.66	1.72	−0.81	0.23	−0.57	9.34	0.79	1	2	5.78
Sb_2S_3	*Pnma* (62)	1.28	1.30	−0.02	−0.01	−0.03	3.89	0.88	2	3	44.94
Bi_2S_3	*Pnma* (62)	1.14	1.14	−0.24	−0.17	−0.41	2.86	0.49	2	1	400.33
BiOI	*P4/nmmS* (129)	1.38	1.49	−0.13	0.00	−0.14	3.75	0.37	9	1	46.32
BiSI	*Pnam* (62)	1.18	1.32	−0.69	0.05	−0.64	4.79	0.53	2	1	29.59
BiSeI	*Pnma* (62)	0.91	1.03	−0.68	0.04	−0.65	5.89	0.25	2	1	26.83
BiSBr	*Pnam* (62)	1.32	1.35	−0.53	−0.11	−0.64	6.21	0.24	2	1	30.10
SbSI	$P2_12_12_1$ (19)	1.28	1.46	−0.23	0.11	−0.11	2.84	0.91	2	2	31.59
SbSI	$Pna2_1$ (33)	1.45	1.60	−0.17	0.11	−0.06	2.06	1.31	2	2	69.72
SbSI	*Pnam* (62)	1.45	1.60	−0.17	0.11	−0.06	2.06	1.25	4	2	69.38
SbSeI	*Pnma* (62)	1.16	1.29	−0.20	0.10	−0.10	4.37	0.59	2	2	43.94
$RbBiS_2$	$R\bar{3}mH$ (166)	1.12	1.47	−0.22	−0.04	−0.27	10.96	0.20	1	2	37.94
$InAlI_4$	$P12_1/m1$ (11)	2.87	2.87	−0.15	0.12	−0.03	1.49	3.90	2	2	19.59
$CaInBr_3$	*Cmcm* (63)	3.12	3.28	−0.04	0.02	−0.02	1.43	0.27	1	2	69.26
KSnSb	$P6_3mc$ (186)	0.18	0.38	−0.08	0.12	0.04	0.25	0.04	0.5	4	2.92
$Cs_3Sb_2I_9$	$P\bar{3}m1$ (164)	1.40	1.41	−0.14	0.20	0.05	2.19	0.25	1	7	13.06
$Cs_3Sb_2I_9$	$P6_3/mmc$ (194)	1.79	1.91	−0.10	0.16	0.06	3.73	0.50	2	2	9.68
$Cs_3Bi_2I_9$	$P6_3/mmc$ (194)	1.90	2.04	−0.46	0.24	−0.22	4.63	1.79	2	3	9.63
$(MA)GeI_3$	$Pm\bar{3}m$ (221)	0.82	0.82	−0.18	0.11	−0.06	0.43	0.51	2	2	6.89
$(MA)SnI_3$	$Pm\bar{3}m$ (221)	0.12	0.12	−0.29	0.05	−0.24	0.12	0.65	1	1	25.57
$(MA)PbI_3$	$Pm\bar{3}m$ (221)	0.31	0.31	−1.12	0.13	−1.00	0.10	0.16	1	1	20.07

R.E. Brandt *et al.*, *MRS Communications* **5**, 265 (2015)
http://dx.doi.org/10.1557/mrc.2015.26

2016: "High-Throughput Experiment": 1 Material per Month



cm CHEMISTRY OF MATERIALS
Article
pubs.acs.org/cm

Searching for "Defect-Tolerant" Photovoltaic Materials: Combined Theoretical and Experimental Screening

Riley E. Brandt,[*,†] Jeremy R. Poindexter,[†] Prashun Gorai,[‡,§] Rachel C. Kurchin,[†] Robert L. Z. Hoye,[†,@] Lea Nienhaus,[†] Mark W. B. Wilson,[†,#] J. Alexander Polizzotti,[†] Raimundas Sereika,[‖] Raimundas Žaltauskas,[‖] Lana C. Lee,[⊥] Judith L. MacManus-Driscoll,[⊥] Moungi Bawendi,[†] Vladan Stevanović,[‡,§] and Tonio Buonassisi[†]

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[‡]Colorado School of Mines, Golden, Colorado 80401, United States
[§]National Renewable Energy Laboratory, Golden, Colorado 80401, United States
[‖]Faculty of Science and Technology, Lithuanian University of Educational Sciences, Vilnius 08106, Lithuania
[⊥]Department of Materials Science and Metallurgy, University of Cambridge, Cambridge CB3 0FE, United Kingdom

Our "high-throughput" search in 2016–2017… 1 material per month, validating predictions for defect-tolerant compounds with large charge-carrier lifetimes

R.E. Brandt *et al.*, *Chemistry of Materials* **29**, 4667 (2017)
https://doi.org/10.1021/acs.chemmater.6b05496

Generative Design Approach

define target properties

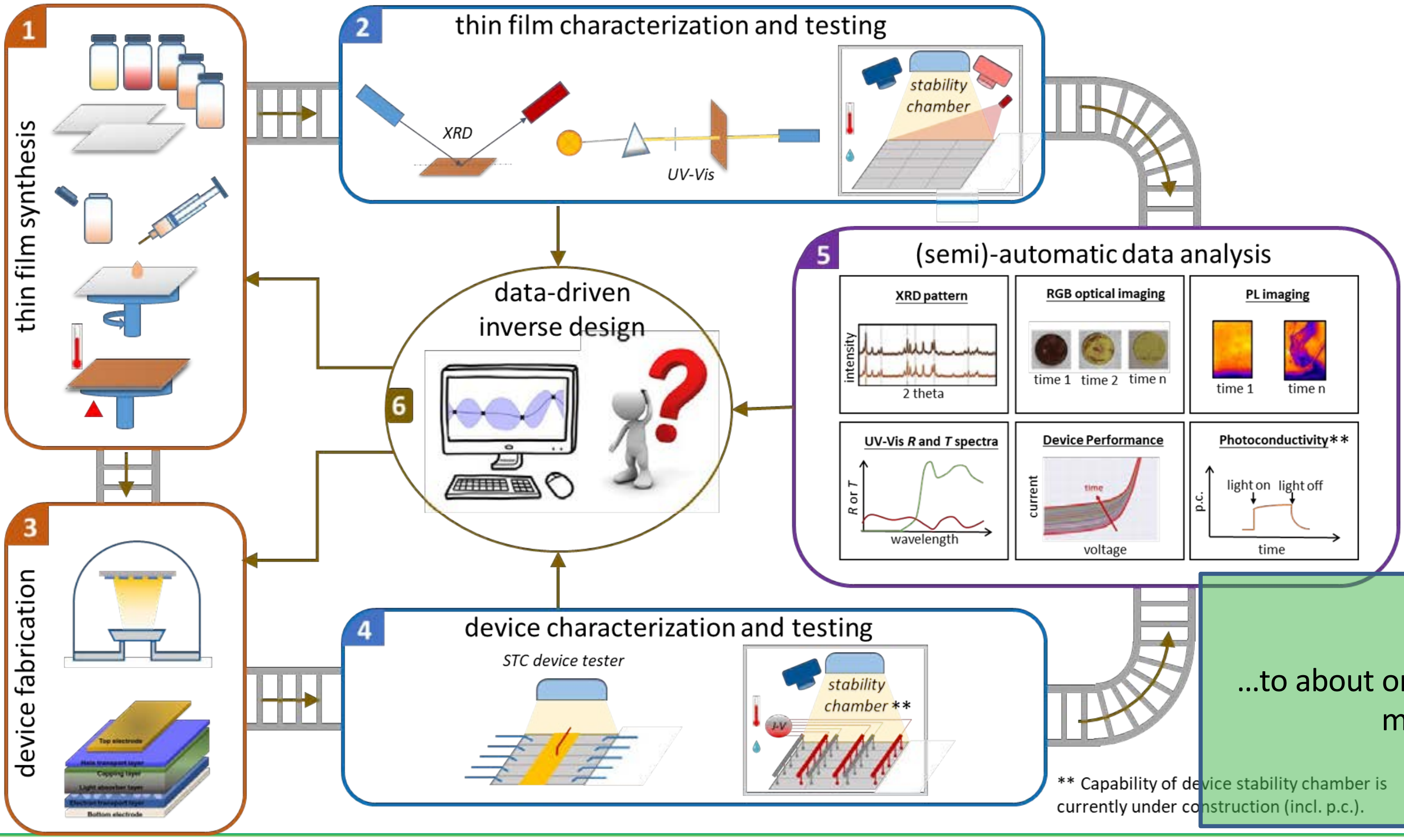
define input variables

search chemical space

identify materials
with target properties

We can increase throughput…

2019: SolTrain: MIT's PV R&D platform

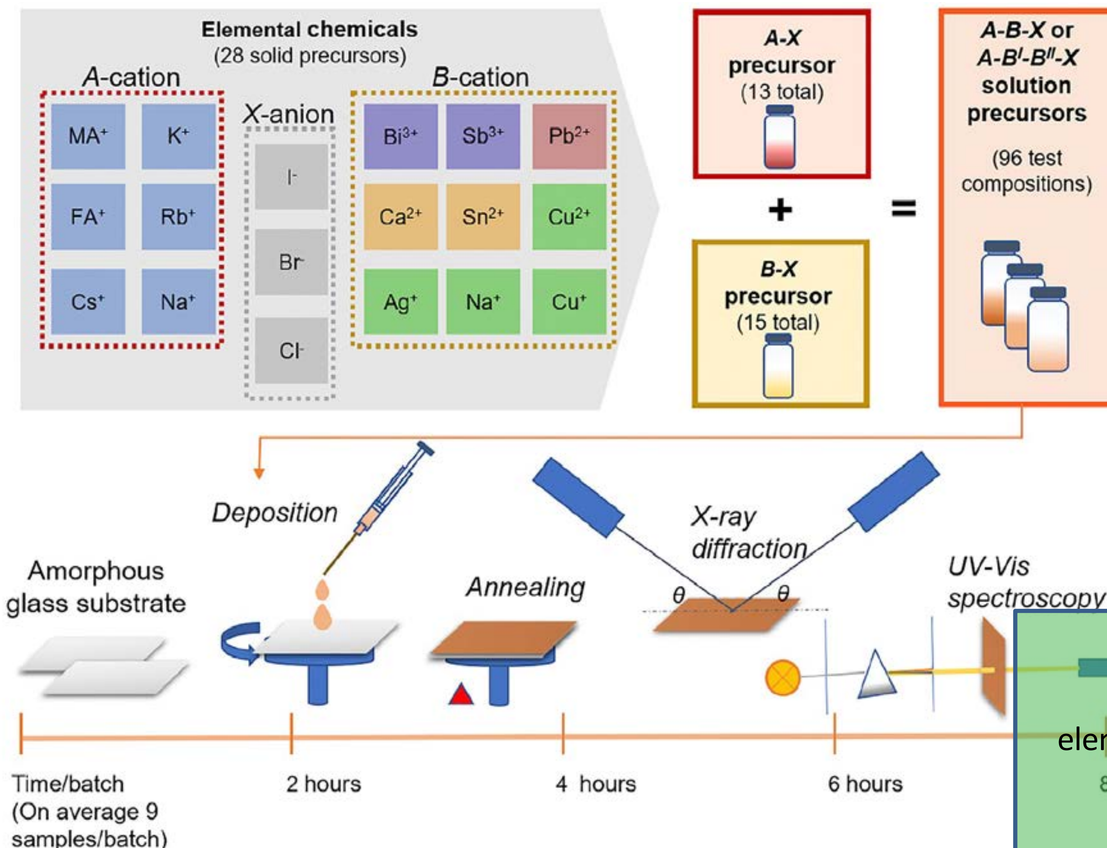


** Capability of device stability chamber is currently under construction (incl. p.c.).

...to about one sample every 5 minutes.

S. Sun *et al.*, *Joule* **3**, 1437 (2019)
https://doi.org/10.1016/j.joule.2019.05.014

2019: Wide elemental range, single platform

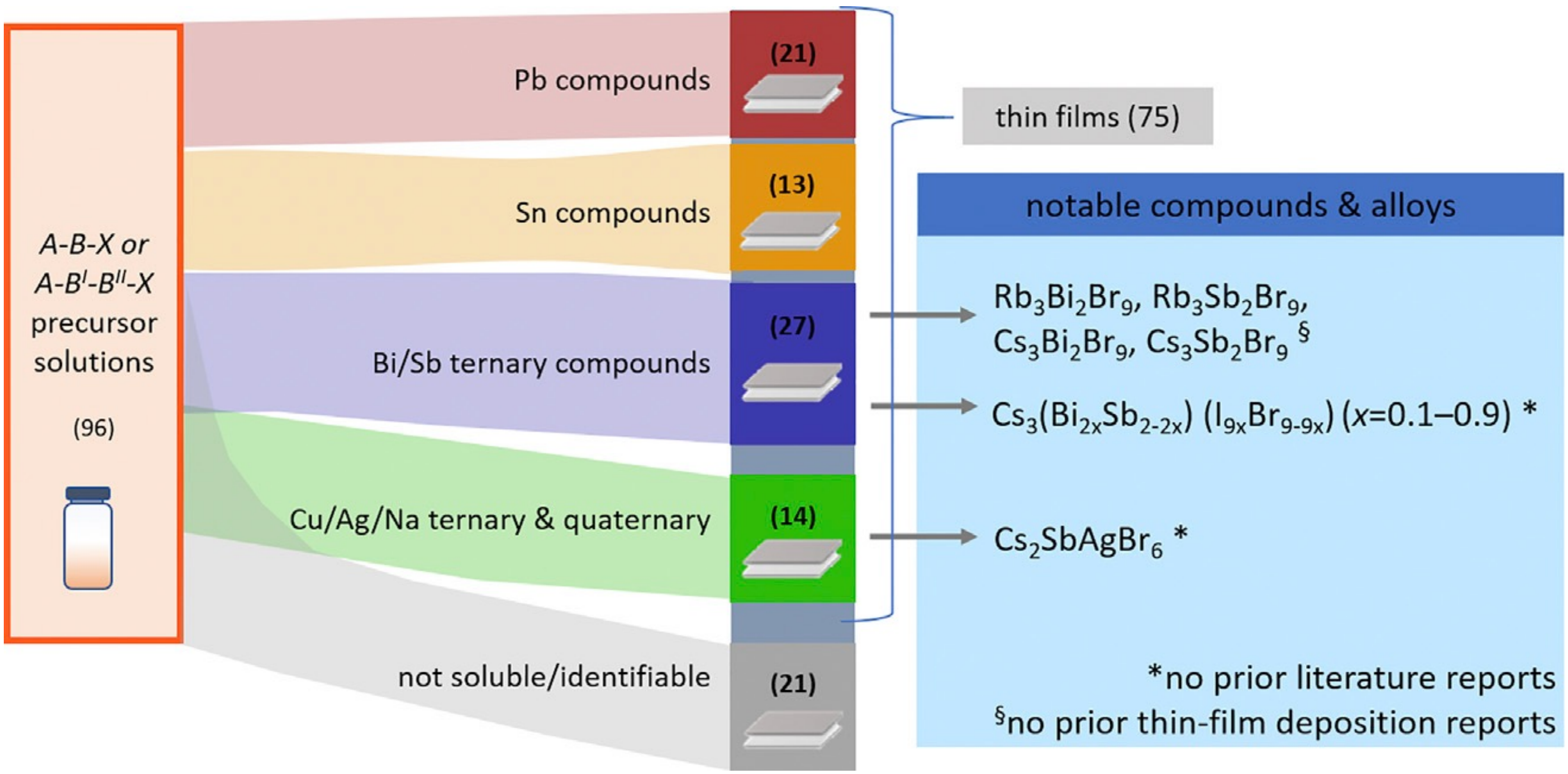


Shijing Sun
MIT; TRI

Mix and match elemental/molecular building blocks

S. Sun *et al.*, *Joule* **3**, 1437 (2019)
https://doi.org/10.1016/j.joule.2019.05.014

2019: Results from 2-mo Campaign

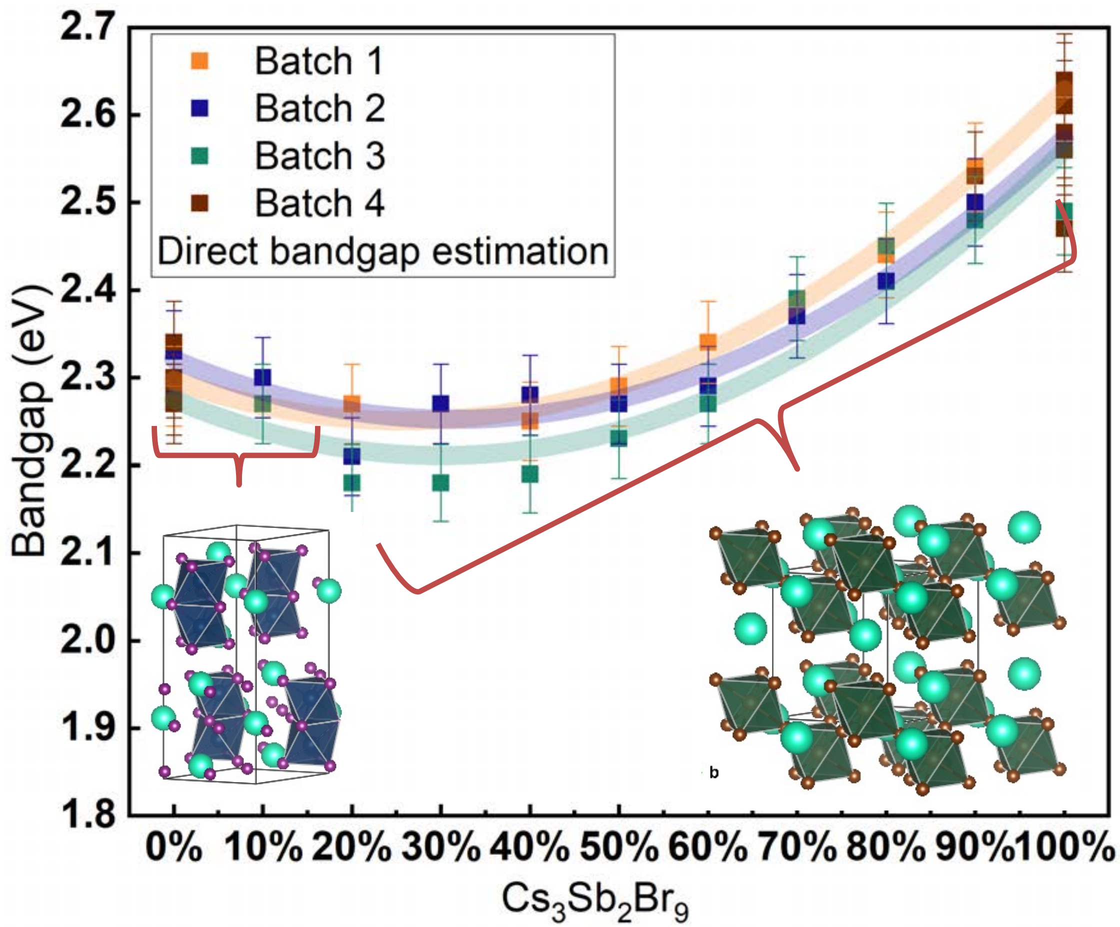


equivalent of 6 journal articles

Discover some new compounds…

S. Sun *et al.*, *Joule* **3**, 1437 (2019)
https://doi.org/10.1016/j.joule.2019.05.014

Bandgap Bowing in $Cs_3(Bi_{1-x}Sb_x)_2(I_{1-x}Br_x)_9$



...and some new science

S. Sun *et al*., *Joule* **3**, 1437 (2019)
https://doi.org/10.1016/j.joule.2019.05.014

But databases and brute-force approaches fail, when you have many (contradicting!) materials properties to simultaneously optimize. New, faster approaches are needed…

PERSPECTIVES

Challenge #1: "Technological applications often demand compounds with what would appear to be a counterintuitive combination of two or more properties. Such compounds harbouring what appears as contradicting attributes are rather difficult to identify and discover."

Invers

with t

Alex Zunger

Abstract | Solid-state chemists have been consistently successful in envisioning and making new compounds, often enlisting the tools of theoretical solid-state physics to explain some of the observed properties of the new materials. Here, a new style of collaboration between theory and experiment is discussed, whereby the desired functionality of the new material is declared first and theoretical

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The properties required to realize a particular device are often known, but the specific materials that harbour such properties are generally unknown and are difficult to identify. The conditions needed for water splitting, the defining qualities of coexisting transparency and conductivity in transparent conductors, and the reason

A. Zunger, *Nat. Rev. Chem.* **2**, 121 (2018)
https://doi.org/10.1038/s41570-018-0121

Generative Design Approach

define target properties

define input variables

run simulation

calculate output parameter(s) of merit

iterate until target reached

The traditional way…

Generative Design Approach

define target properties

define input variables

use ML surrogate model

- solve directly
- Use PSO

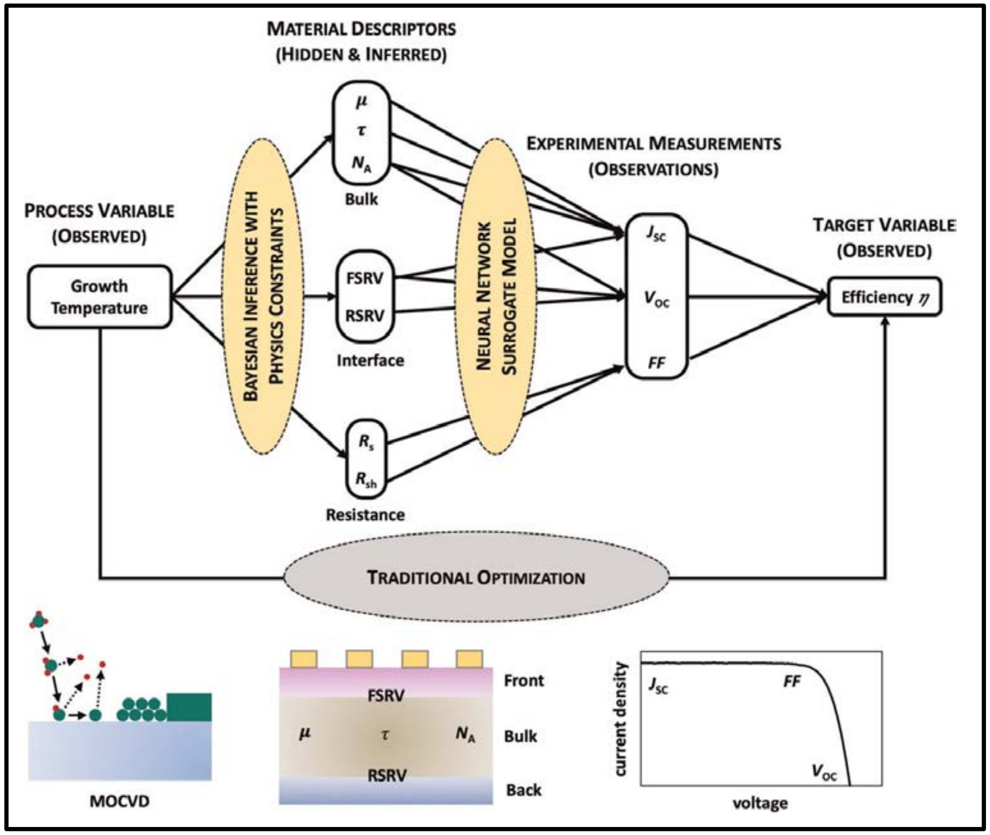
achieve output parameter(s) of merit

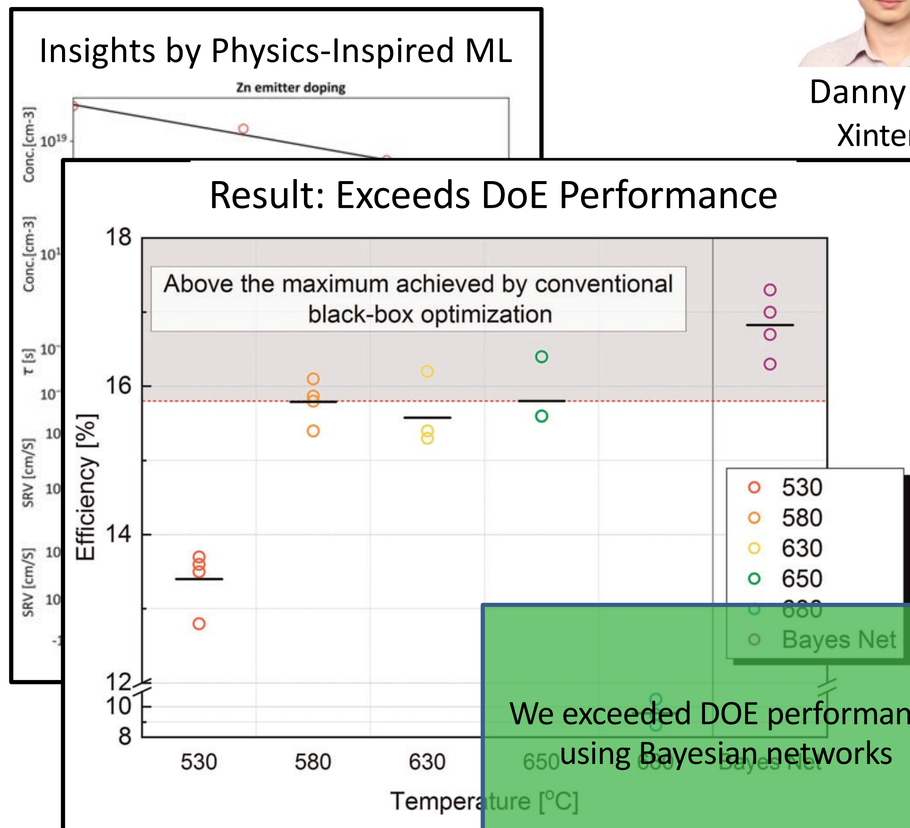
...and an emergent way with the diffusion of machine learning in materials research

SMART: Singapore-MIT Alliance for Research & Technology

Here’s where I spent much of the last 6 years…

Implementing Heuristics into Bayesian Inference





We exceeded DOE performance using Bayesian networks

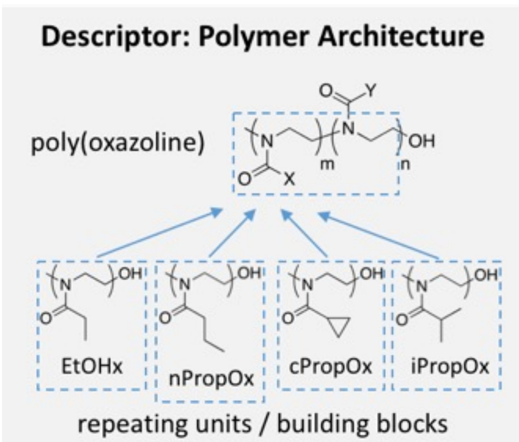
Z. Ren, F. Oviedo *et al.*, *npj Computational Materials* **6**, 9 (2020)
https://doi.org/10.1038/s41524-020-0277-x

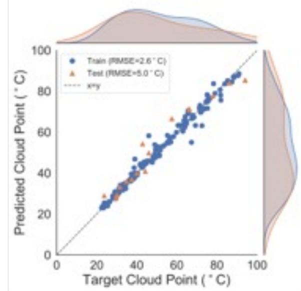
Agency for Science, Technology & Advanced Research (A*STAR)

I took a year leave of absence to start up a $18M, 5-year program at A*STAR, called Accelerated Materials Development for Manufacturing (AMDM).

- Polymers
- Nanoparticles
- Integrated Circuits
- Metals
- Magnetic Materials

Polymer Inverse Design



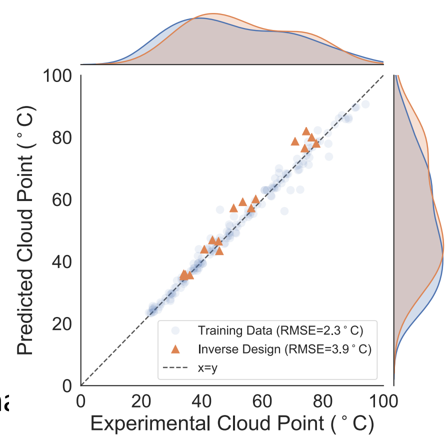


Model Training

Gradient Boosting w Decision Trees

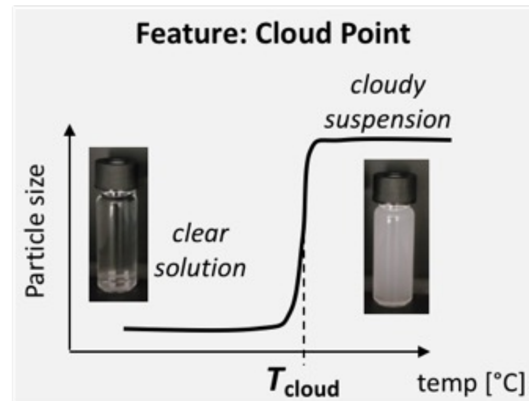
Inverse Design

Particle Swarm Optimization



Here, a trained regressor could be explored using particle swarm optimization, to identify combinations of input conditions satisfying a user-defined target

Jatin Kumar
A*STAR; Xinterra



Created 17 new polymers with user-defined properties *via* inverse design

J. Kumar *et al.*, *npj Comp. Mat.* **5**, 73 (2019)
https://doi.org/10.1038/s41524-019-0209-9

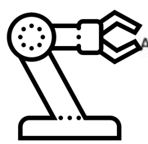
Buona

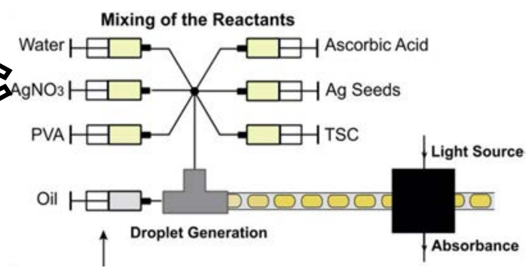
Accelerated Materials Laboratory for **Sustainability**

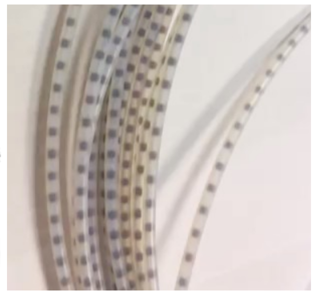
Identify Nanoparticle Process Recipe in 2 weeks (compared to 1 yr)

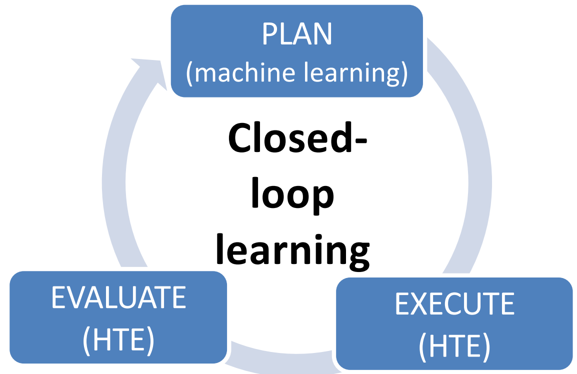
Flor M.B.
NUS

- ➢ **High-throughput synthesis (microfluidics)**



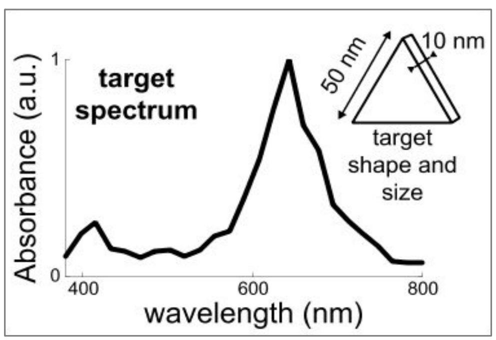




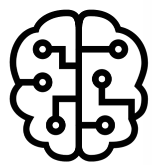


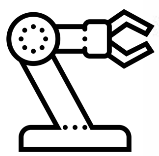
Similar, but for silver nanoparticles. We ran BO and a NN in parallel, to both optimize and regress (toward inverse design).

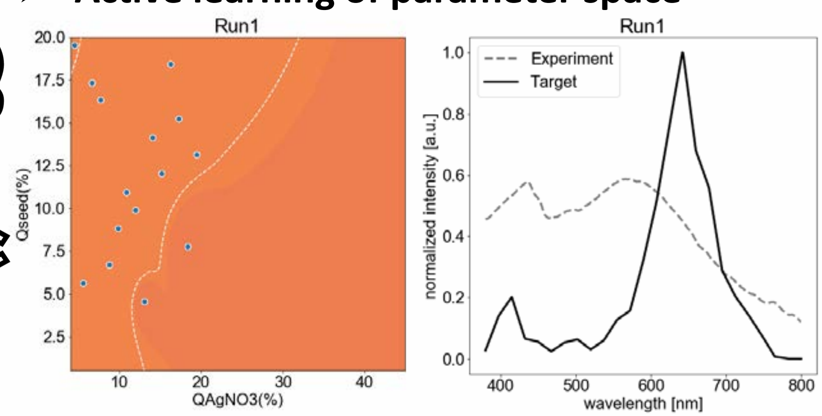
- ➢ **Define Target (simulation)**

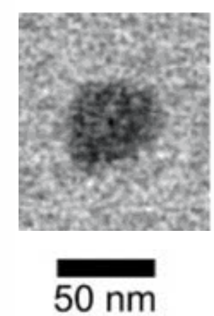


- ➢ **Active learning of parameter space**







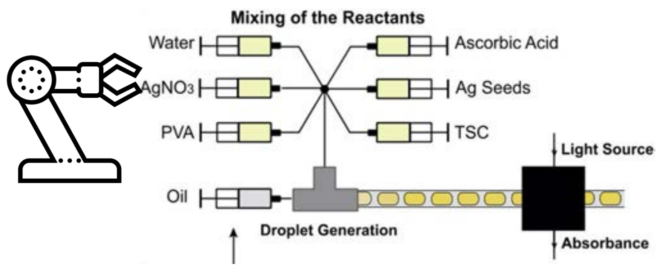


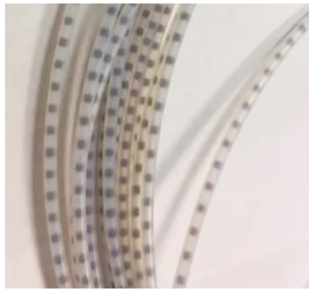
F. Mekki-Berrada, Z. Ren, T. Huang *et al.*, *npj Comp. Mat.* **7**, 55 (2021)
https://doi.org/10.1038/s41524-021-00520-w

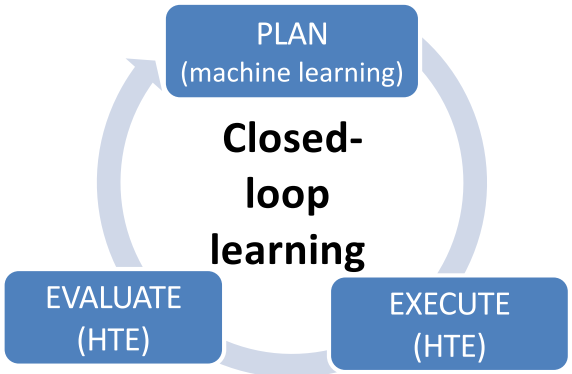
20220815

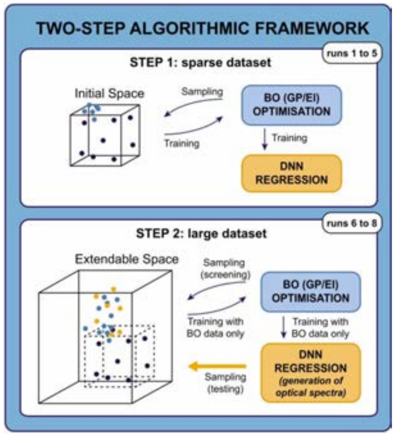
Identify Nanoparticle Process Recipe in 2 weeks (compared to 1 yr)

- High-throughput synthesis (microfluidics)

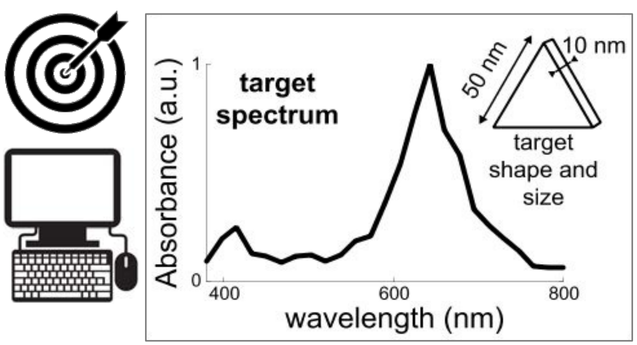




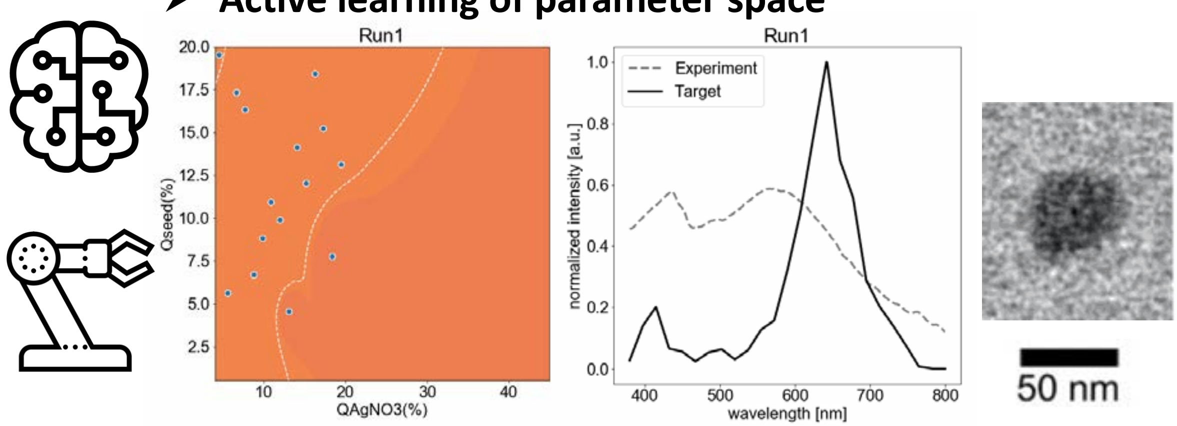




- Define Target (simulation)



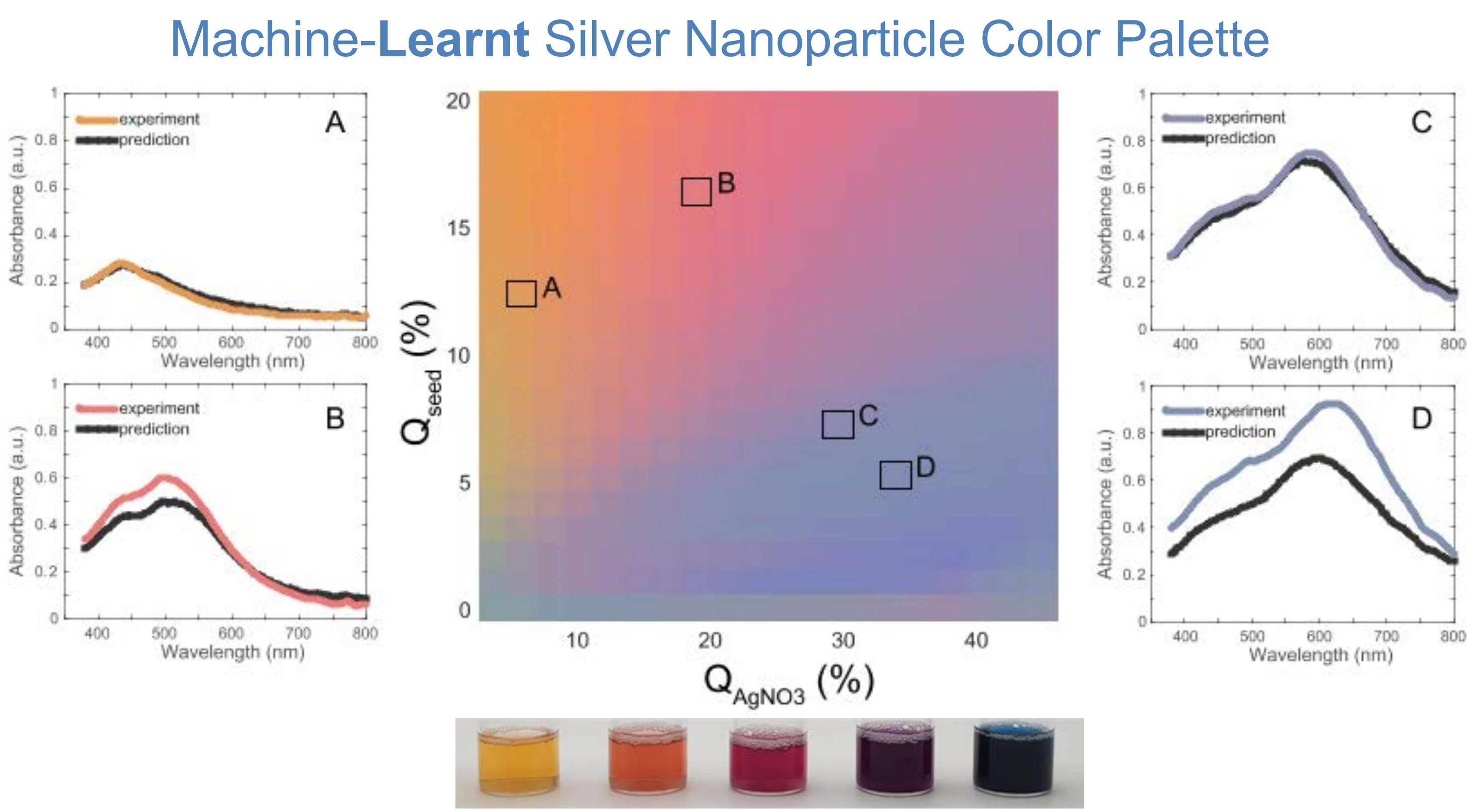
- Active learning of parameter space



F. Mekki-Berrada, Z. Ren, T. Huang *et al.*, *npj Comp. Mat.* **7**, 55 (2021)
https://doi.org/10.1038/s41524-021-00520-w

20220815

Identify Nanoparticle Process Recipe in 2 weeks (compared to 1 yr)



Inverse design with trained regressors… almost like a lookup table.

F. Mekki-Berrada, Z. Ren, T. Huang *et al.*, *npj Comp. Mat.* **7**, 55 (2021)
https://doi.org/10.1038/s41524-021-00520-w

20220815

Accelerated Materials Laboratory for **Sustainability**

PERSPECTIVES

Challenge #2: "Because the effective interactions used as input are generally not expressible (or mappable) in terms of the periodic table, there is generally no recognizable rational path between model Hamiltonian predictions and the realization of actual materials. In other words, the theory is not <u>invertible</u>."

Invers… with t…

Alex Zunger

Abstract | Solid-state chemists have been consistently successful in envisioning and making new compounds, often enlisting the tools of theoretical solid-state physics to explain some of the observed properties of the new materials. Here, a new style of collaboration between theory and experiment is discussed, whereby the desired functionality of the new material is declared first and theoretical

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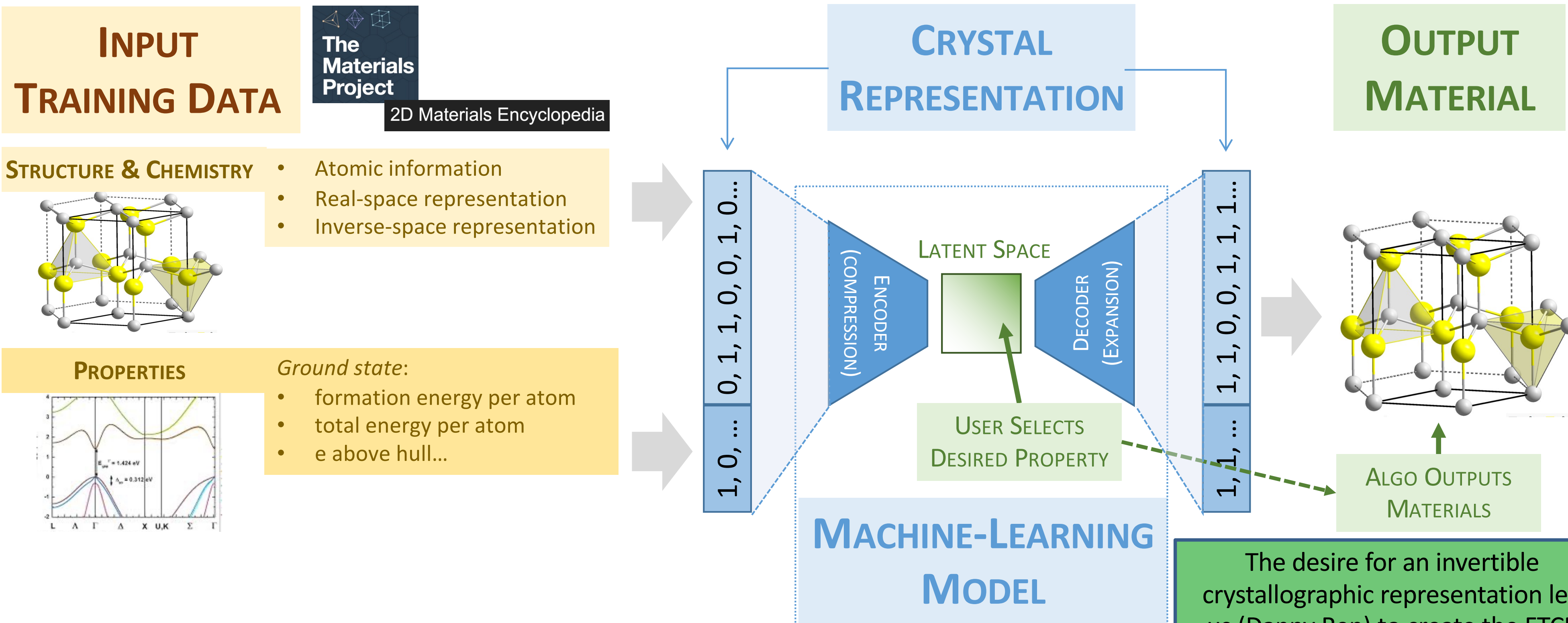
A. Zunger, *Nat. Rev. Chem.* **2**, 121 (2018)
https://doi.org/10.1038/s41570-018-0121

Accelerated
Materials
Laboratory for
Sustainability

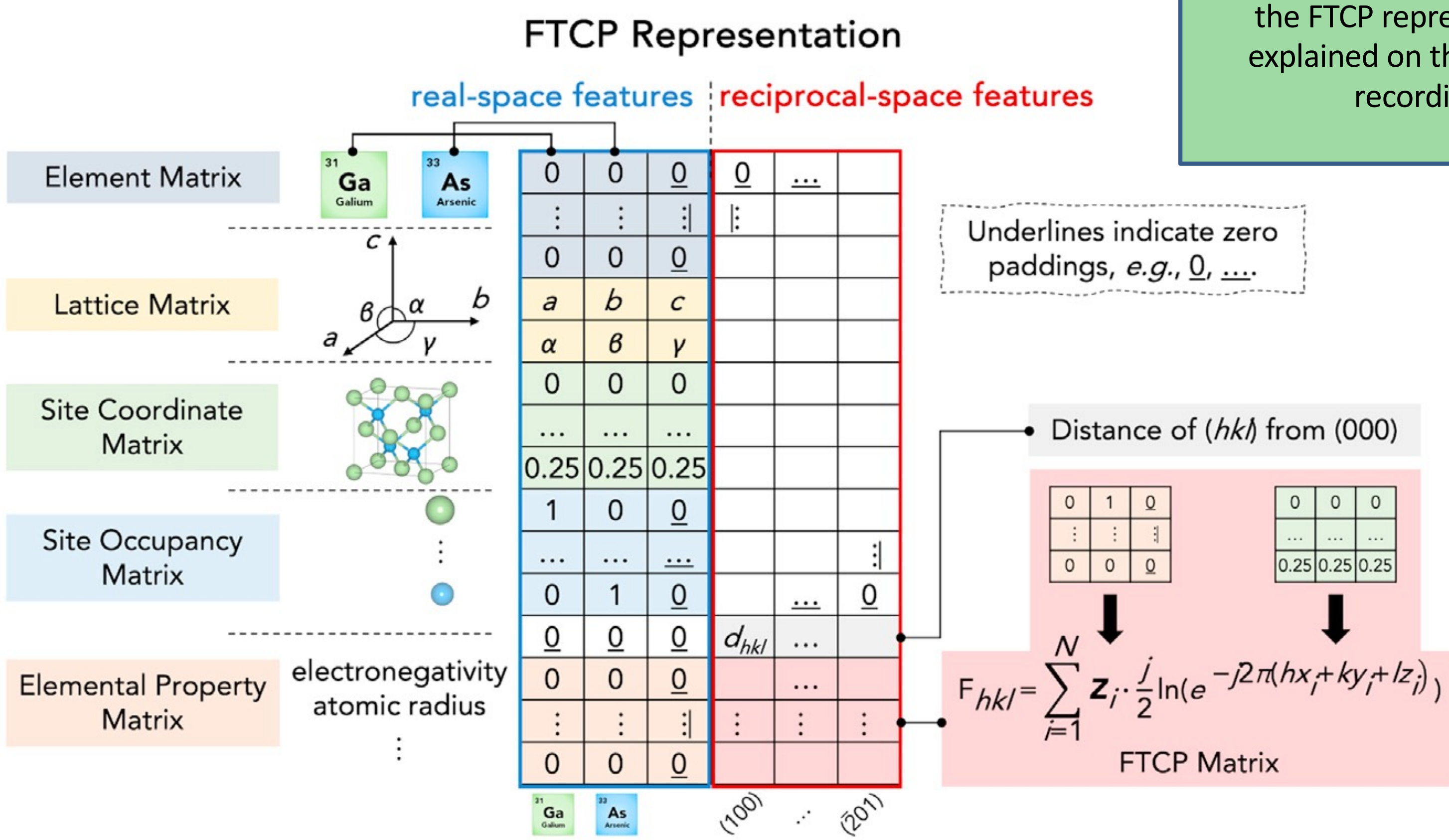
Inverse Design using FTCP



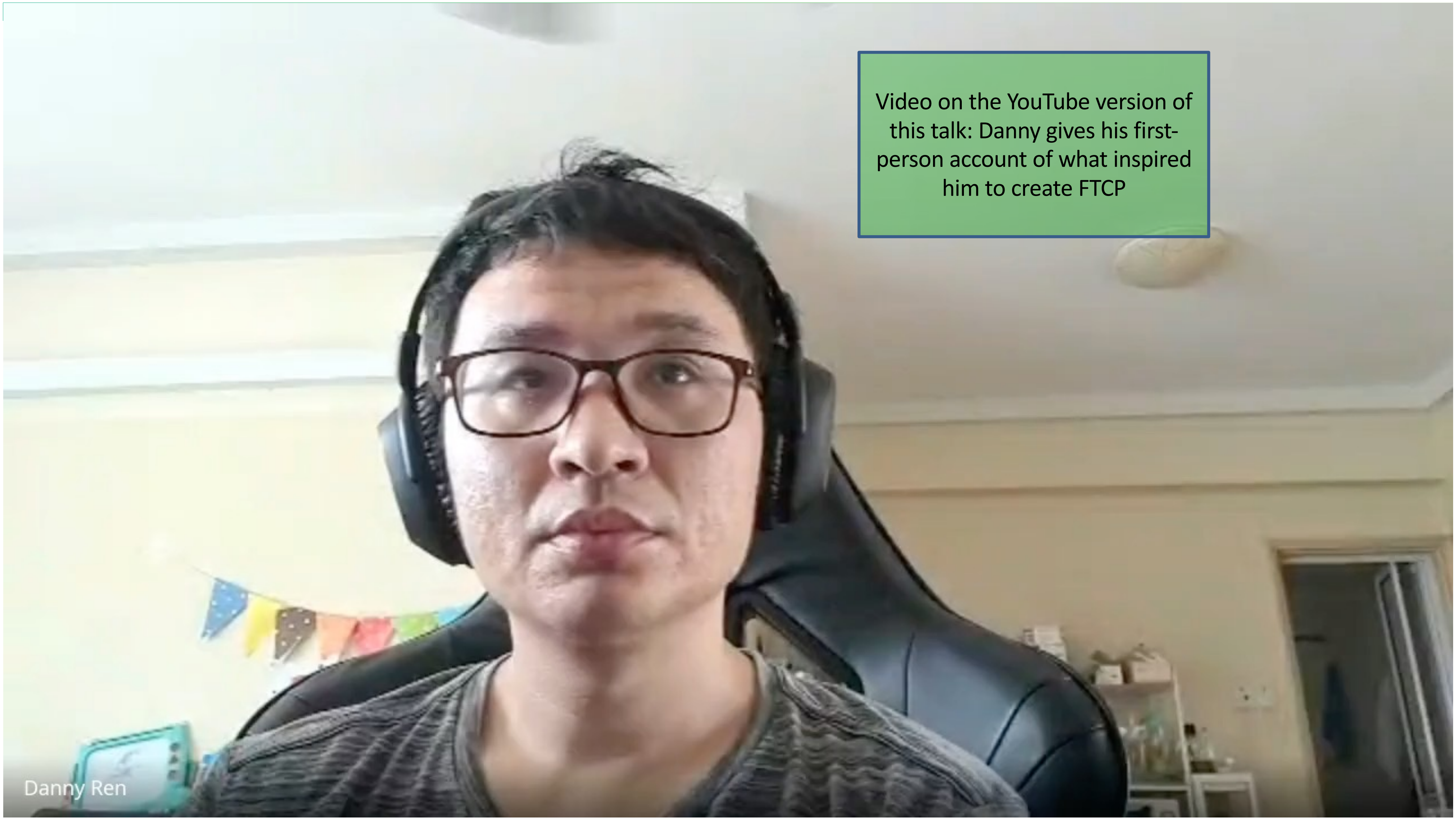
The desire for an invertible crystallographic representation led us (Danny Ren) to create the FTCP materials representation, which when combined with a VAE, enables general inverse design.

Z. Ren, S.I.P. Tian *et al.*, *Matter* **5**, P314 (2022)
https://doi.org/10.1016/j.matt.2021.11.032

FTCP Representation



Here are the different pieces of the FTCP representation, explained on the YouTube recording.



Video on the YouTube version of this talk: Danny gives his first-person account of what inspired him to create FTCP

This is the big one. Many groups out there trying to predict synthesizability, synthesis routes, metastability…

PERSPECTIVES

Challenge #3: "because the total electron and ion energy of the system is generally not computed or optimized with respect to the structural degrees of freedom, it is difficult to assess whether the predicted properties (such as exotic superconductivity and quantum spin liquids) will be found in <u>stable</u> (or nearly stable) recognizable compounds"

Invers… with t…

Alex Zunge…

Abstract | Solid-state chemists have been consistently successful in envisioning and making new compounds, often enlisting the tools of theoretical solid-state physics to explain some of the observed properties of the new materials. Here, a new style of collaboration between theory and experiment is discussed, whereby the desired functionality of the new material is declared first and theoretical

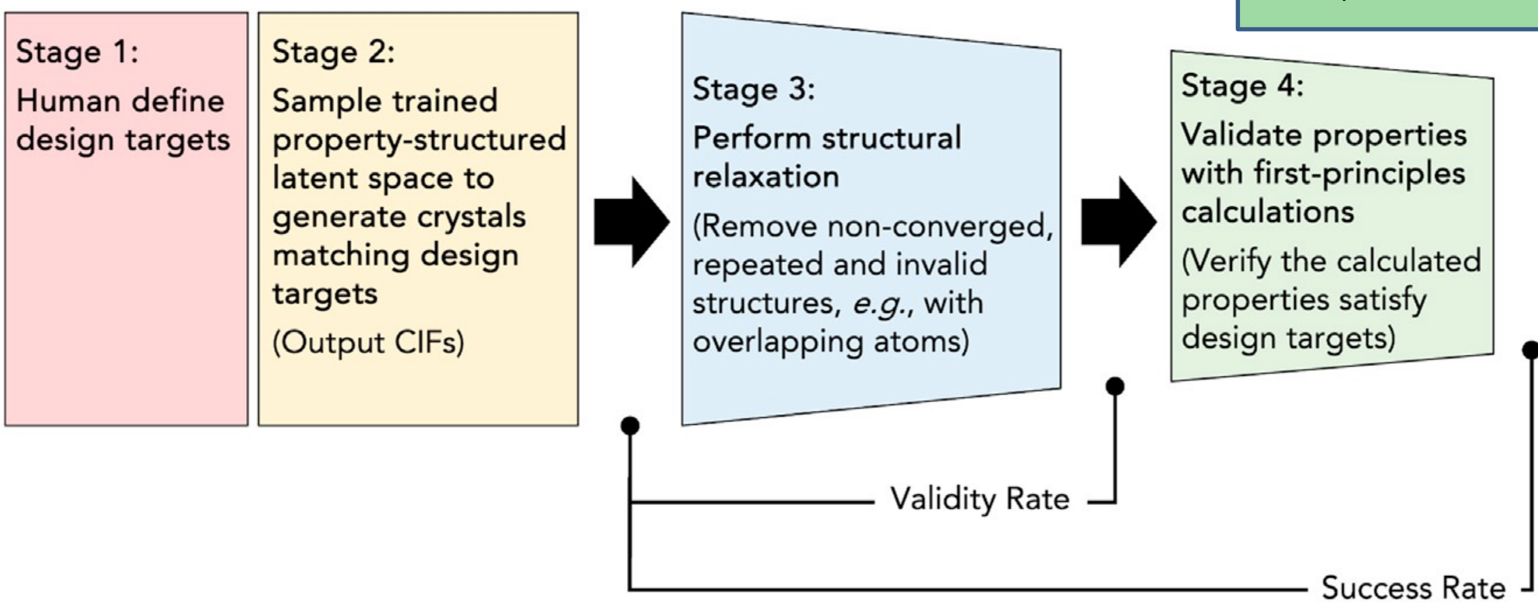
…n ACSs and …question …sed- …organic matter …ode' of …ul) relations? …ealize a …wn, but the specific materials that harbour such properties are generally unknown and are difficult to identify. The conditions needed for water splitting, the defining qualities of coexisting transparency and conductivity in transparent conductors, and the reason

A. Zunger, *Nat. Rev. Chem.* **2**, 121 (2018)
https://doi.org/10.1038/s41570-018-0121

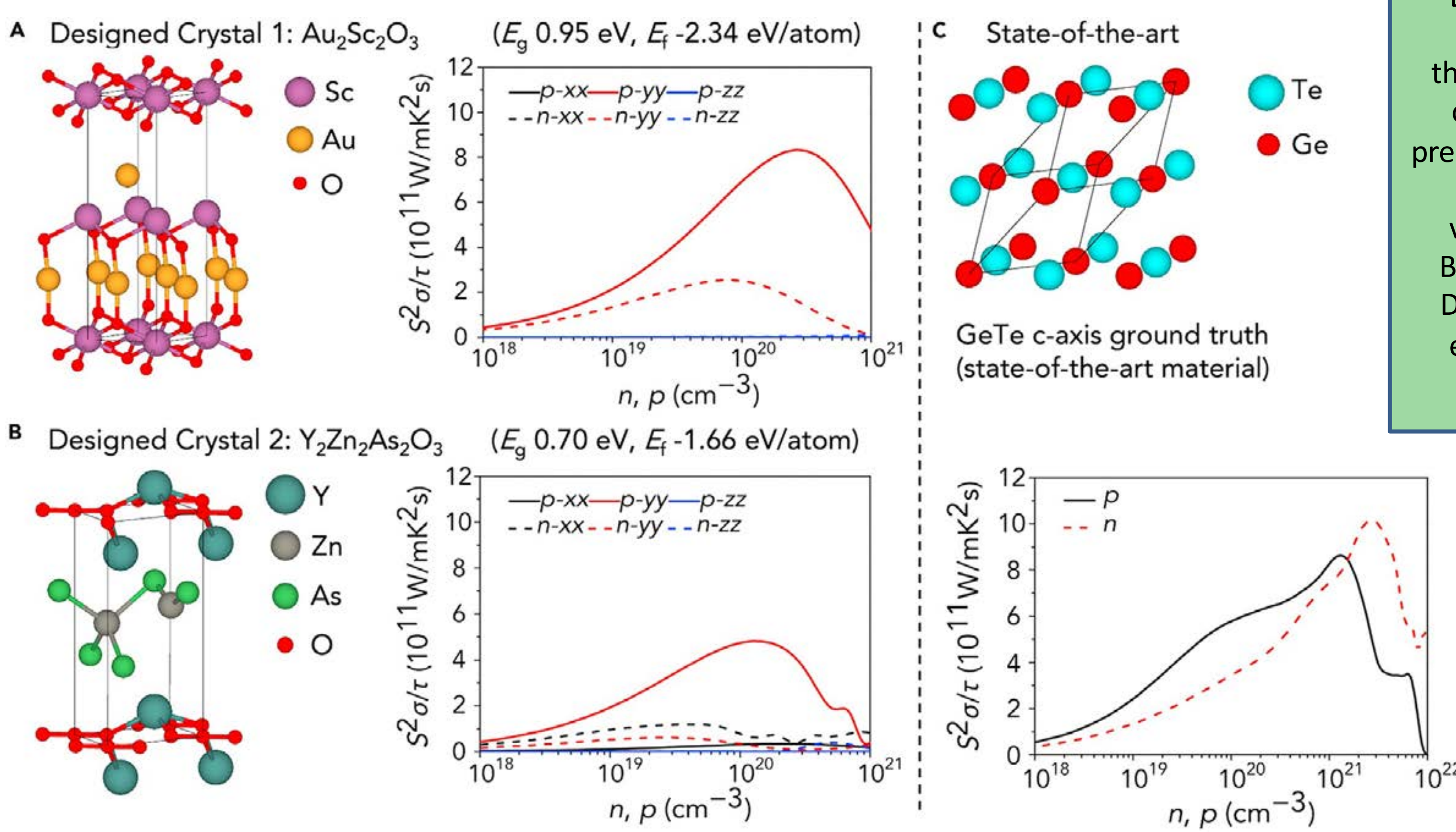
Accelerated Materials Laboratory for **Sustainability**

Open Challenges

Our workflow from the FTCP paper, trying to filter out compounds that cannot be synthesized, so we don't waste experimental bandwidth.



Examples

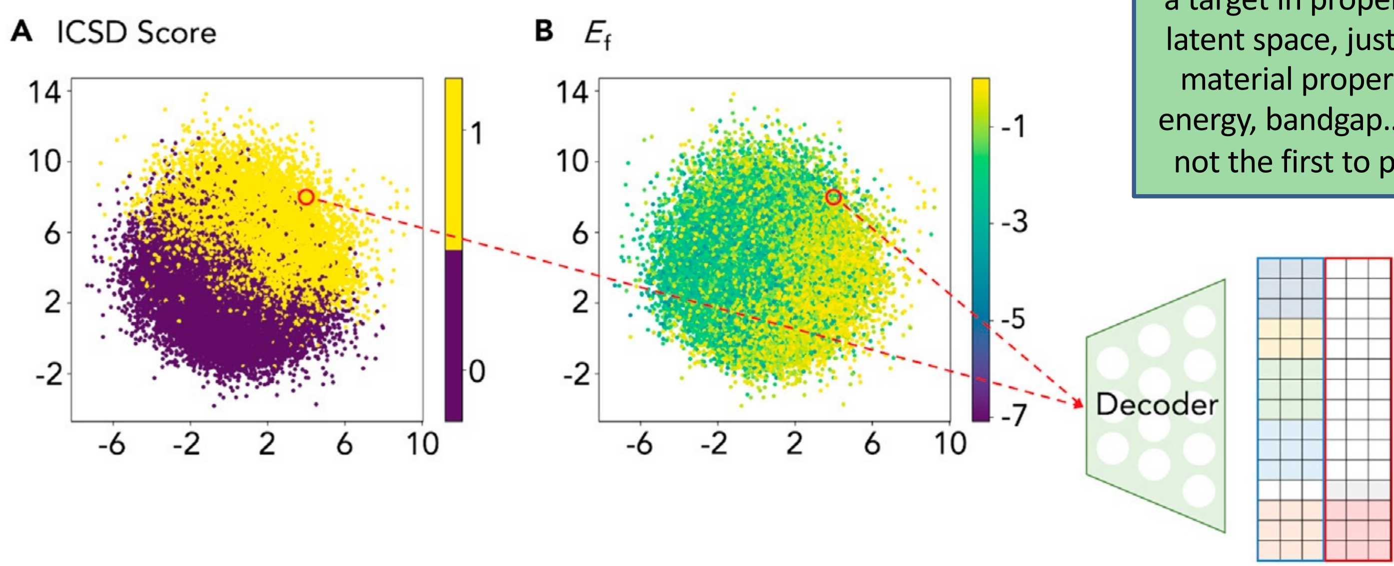


Examples of candidate thermoelectric compounds predicted by FTCP that were validated by BoltzTraP and DFT… but not experiment.

Z. Ren, S.I.P. Tian *et al.*, *Matter* **5**, P314 (2022)
https://doi.org/10.1016/j.matt.2021.11.032

"ICSD Score" as a Synthesizability Metric

One approach to predict synthesizability: How closely does the candidate resemble a compound in the ICSD (*i.e.*, already synthesized)? This can be a target in property-segmented latent space, just like any other material property (formation energy, bandgap…). (*NB*: We are not the first to propose this…)



Z. Ren, S.I.P. Tian *et al.*, *Matter* **5**, P314 (2022)
https://doi.org/10.1016/j.matt.2021.11.032

Materials representations: Video! Isaac presents his new paper, "What information is necessary & sufficient to predict materials properties?"

What Information is Necessary and Sufficient to Predict Materials Properties using Machine Learning?

Siyu Isaac Parker Tian, Aron Walsh, Zekun Ren, Qianxiao Li, Tonio Buonassisi

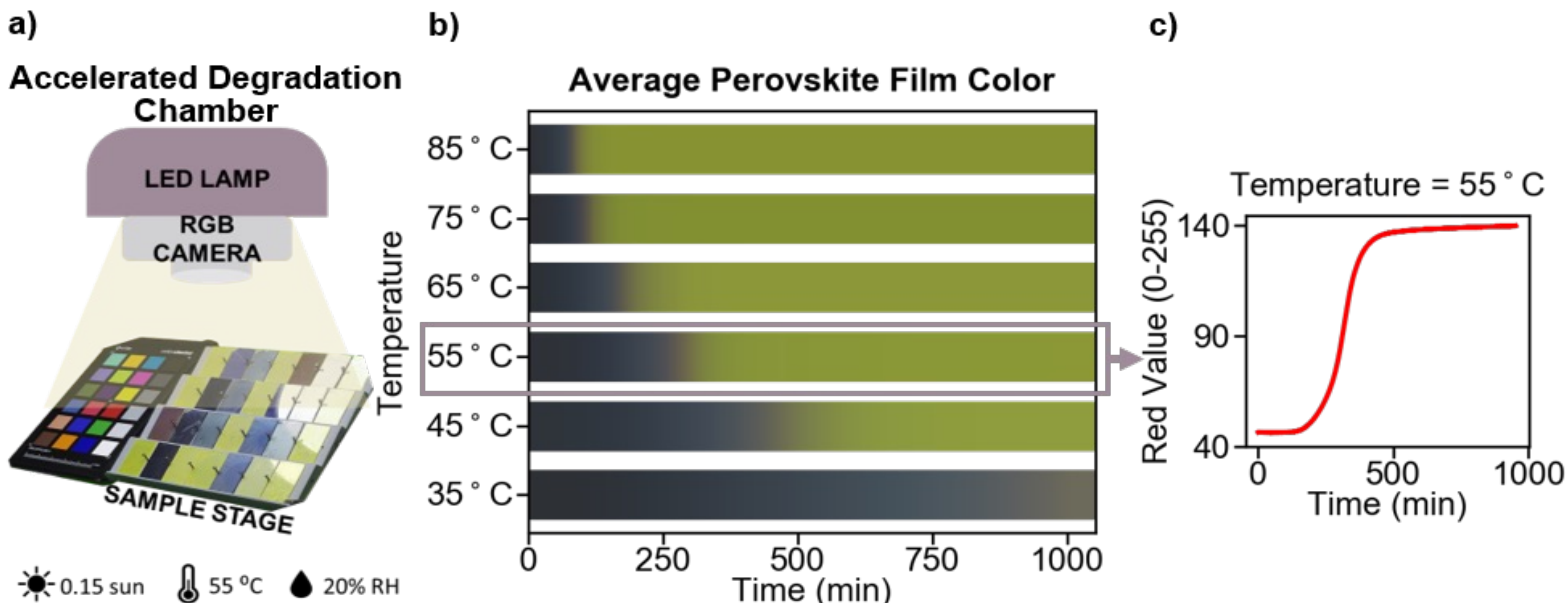
S.I.P. Tian *et al.*, arXiv (2022)
https://arxiv.org/abs/2206.04968

Here's one of the earlier conversations about that paper.

I didn't have time to cover this during the talk, so here are some bonus slides…

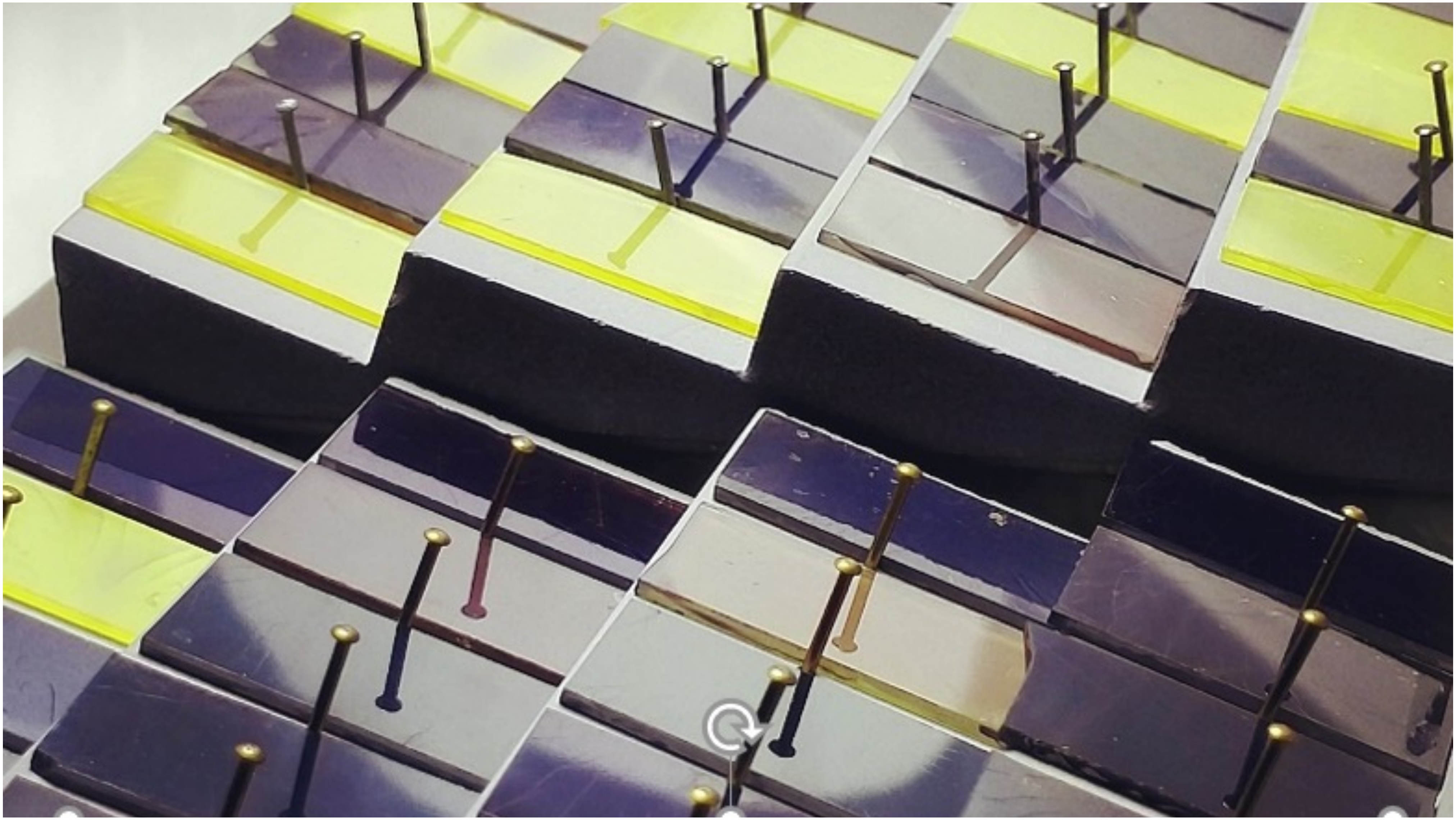
Gaining Human Trust

Study of Perovskite Film Degradation as a Function of Temperature

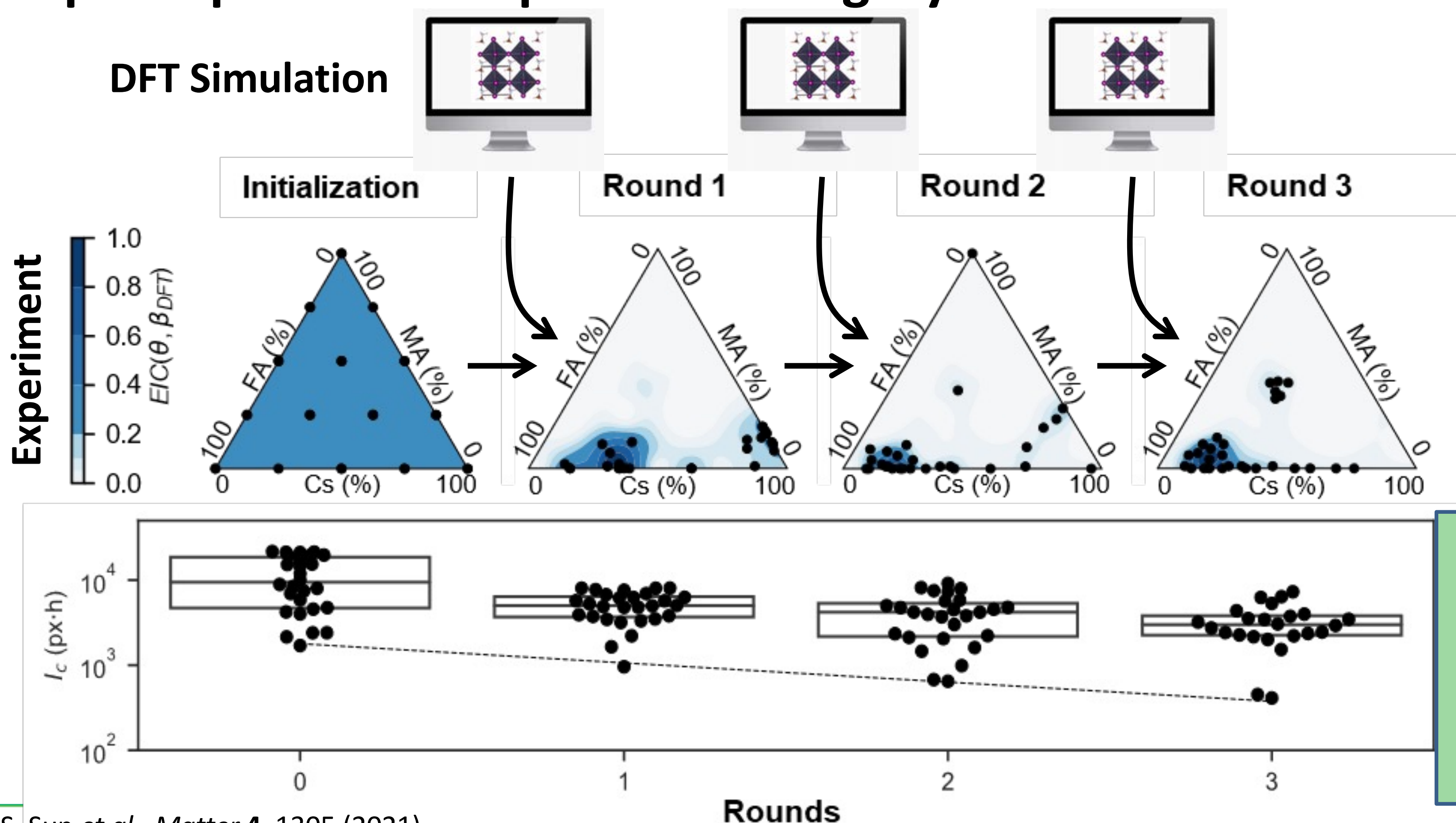


Here's an example set of experiments, whereby scientific knowledge can be input and extracted from ML-guided experiments. Here, we used color-calibrated, camera-based imaging to detect the onset of perovskite (MAPI) film degradation.

R.R. Naik *et al.*, *npj Computational Materials* **8**, 72 (2022)
https://doi.org/10.1038/s41524-022-00751-5 Buonassisi — MIT — 20220815



Step 2: Optimize Composition Using Hybrid Model

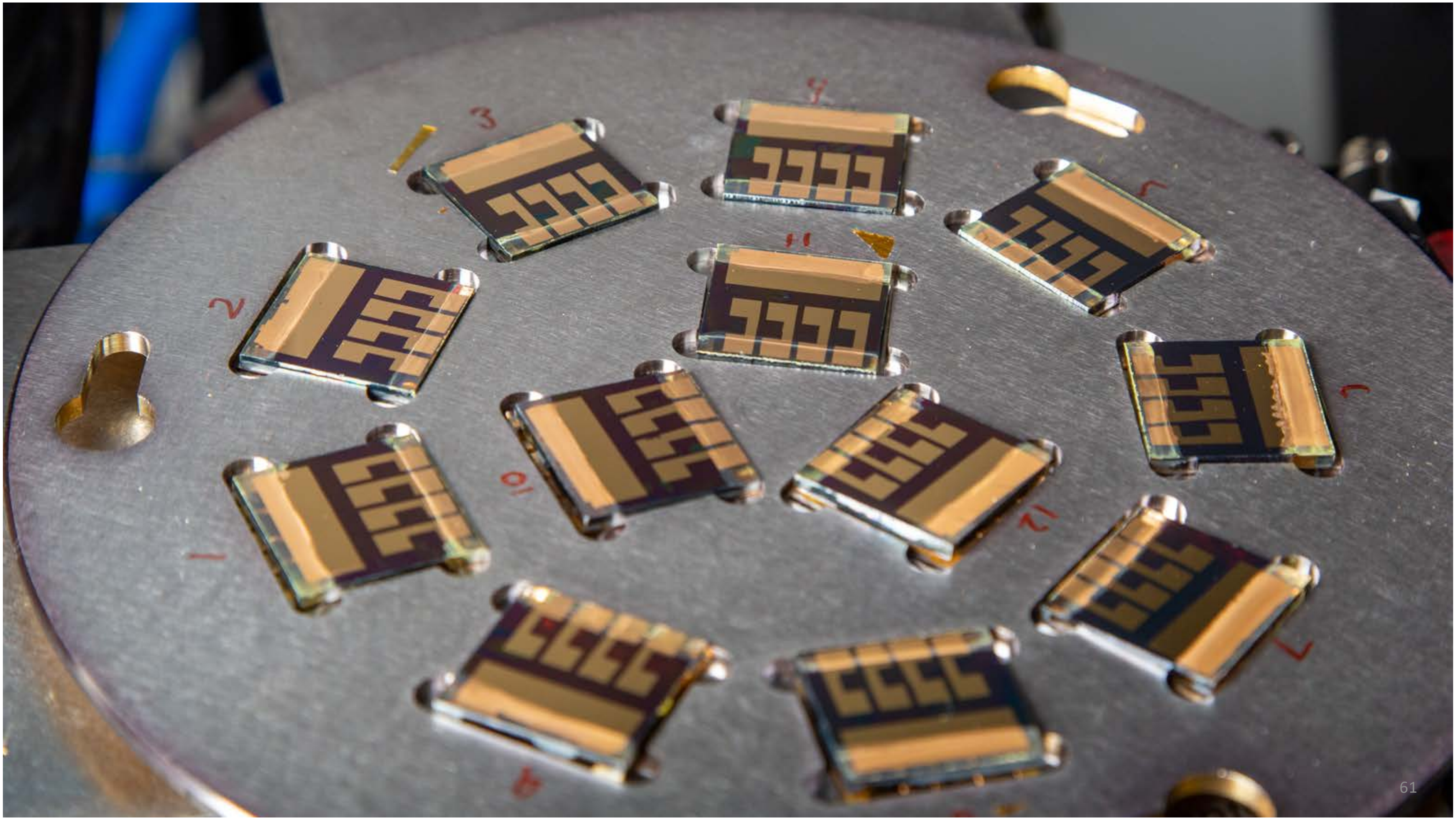


Shijing SUN

Armi TIIHONEN

We used interpretable DFT data as a “soft constraint” to nudge the Bayesian optimization cycles, toward identifying more stable perovskite compositions.

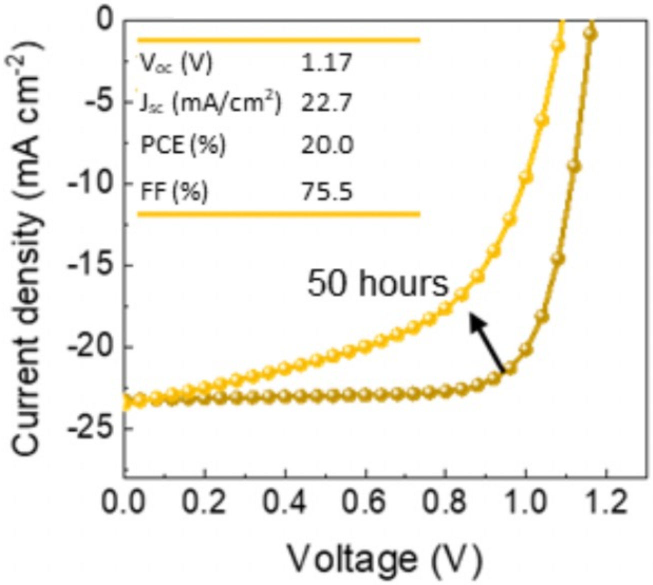
S. Sun *et al.*, *Matter* **4**, 1305 (2021)
https://doi.org/10.1016/j.matt.2021.01.008



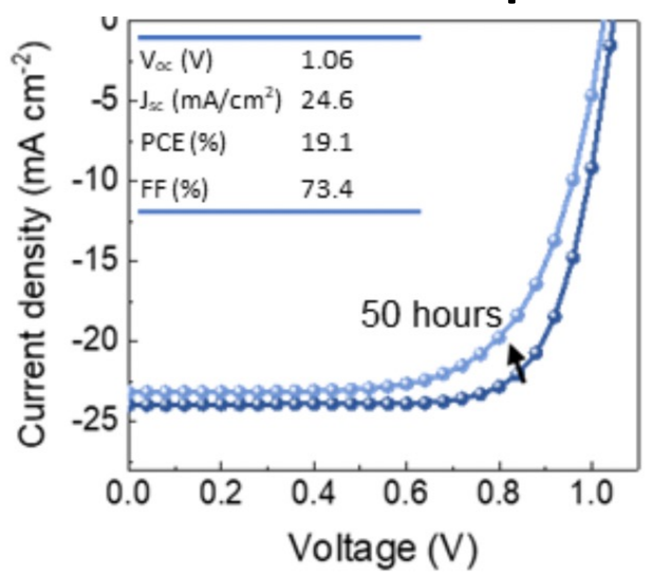
Bonus: Demonstrate Scale-Up with Fewer Attempts

Device fabrication performed by the team of Christoph Brabec

State-of-the-Art



ML-Informed Composition



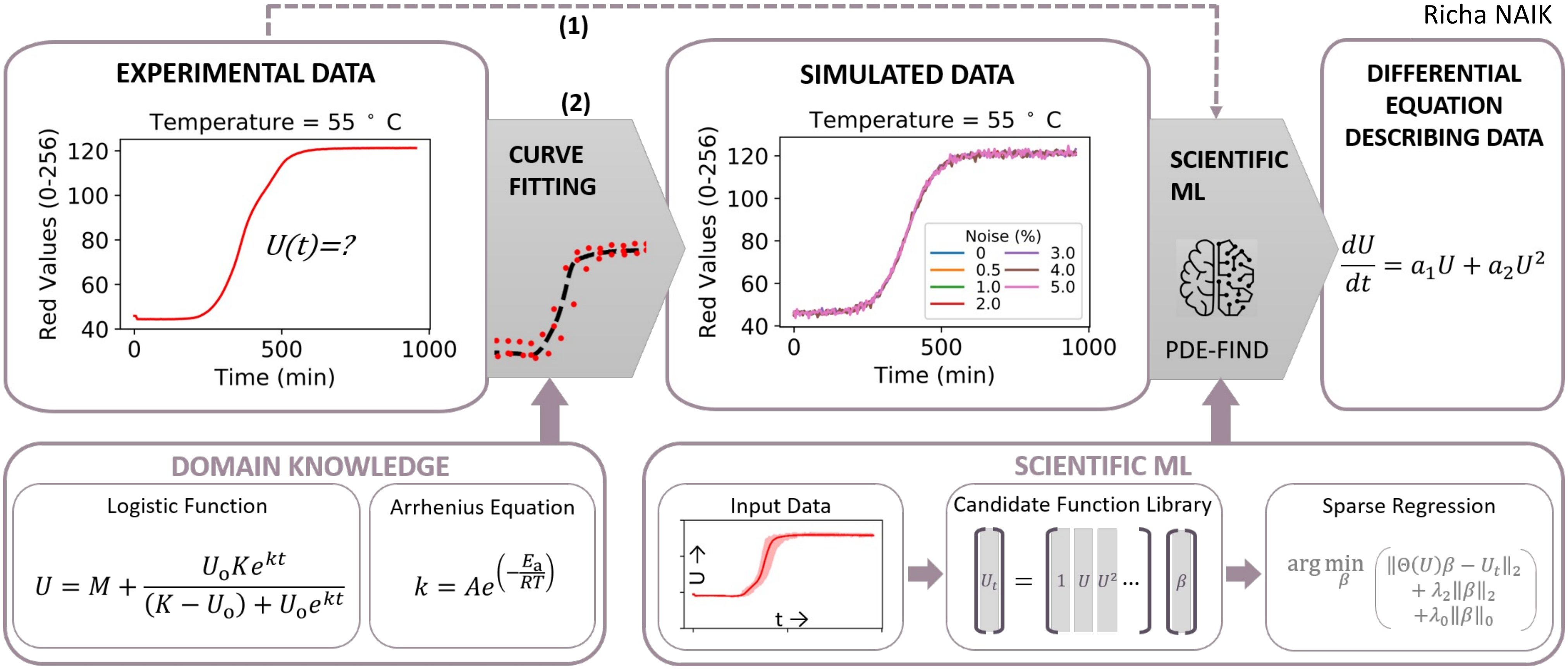
Environmental testing: 50 hrs under 85% RH / 85°C in air

The pandemic gave us an opportunity to cement new collaborations. Christoph Brabec' team in Germany made devices, which confirmed that our ML-guided composition was considerably more stable than the prior SOTA composition, indicating that this film-based proxy measurement translates into full devices.

S. Sun *et al.*, *Matter* **4**, 1305 (2021)
https://doi.org/10.1016/j.matt.2021.01.008

Extract Knowledge: Infer Root Cause(s) of Degradation

Richa NAIK



R.R. Naik *et al.*, *npj Computational Materials* **8**, 72 (2022)
https://doi.org/10.1038/s41524-022-00751-5 Buonassisi — MIT — 20220815

We used sparse regression to identify the equations governing MAPI degradation.

Human Interpretation

$$\frac{dU}{dt} = a_0 + a_1 U + a_2 U^2$$

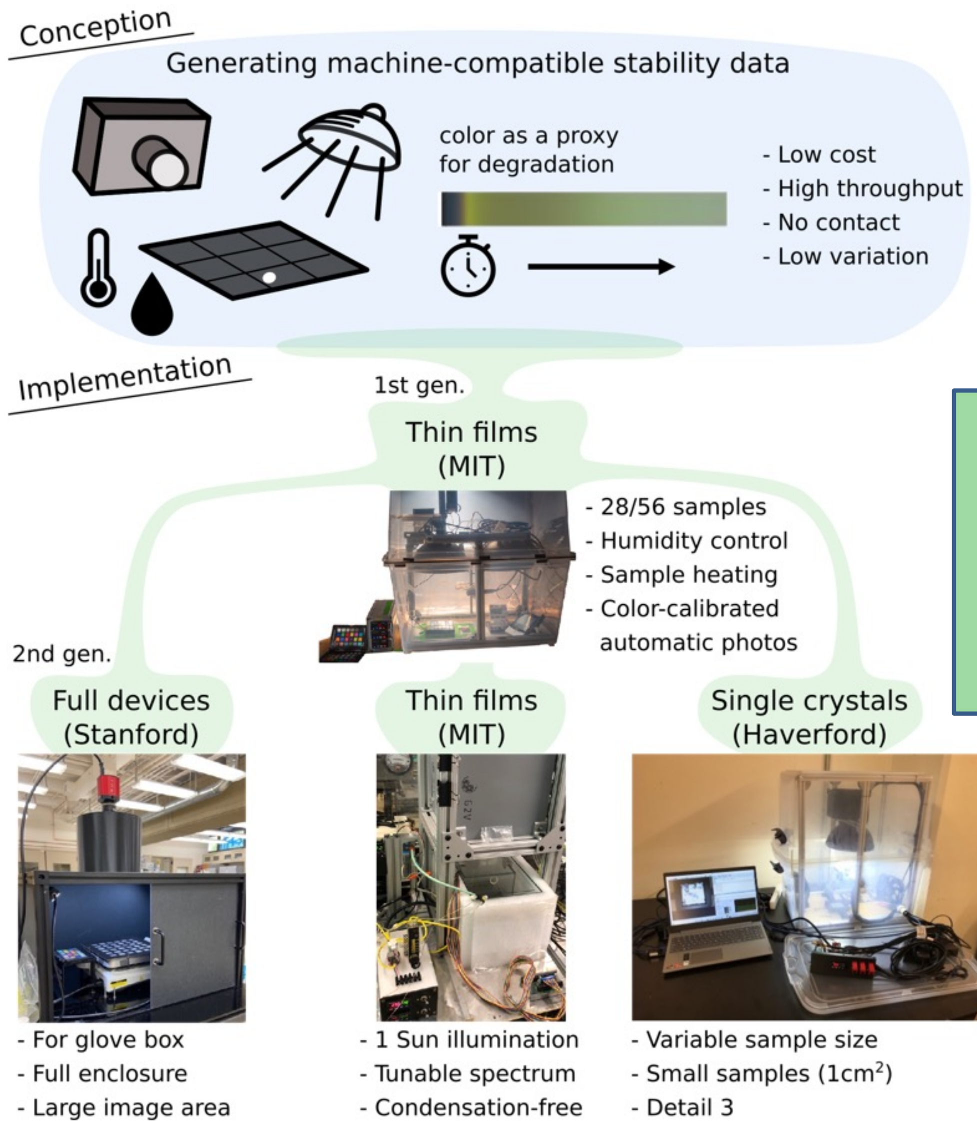
The identified equation corresponds to an autocatalytic reaction — meaning that once the reaction starts, it is hard to stop. The trick is to avoid nucleation sites that can promote decomposition, suggesting greater film (+precursor) purity is important. Interestingly, OLEDs underwent similar learning, to achieve commercial displays.

<u>OLEDs suggest a pathway for perovskites:</u>

- Hermetically seal the device
- Avoid impurities (*i.e.*, nucleation points for phase transformation) in the sealed devices.

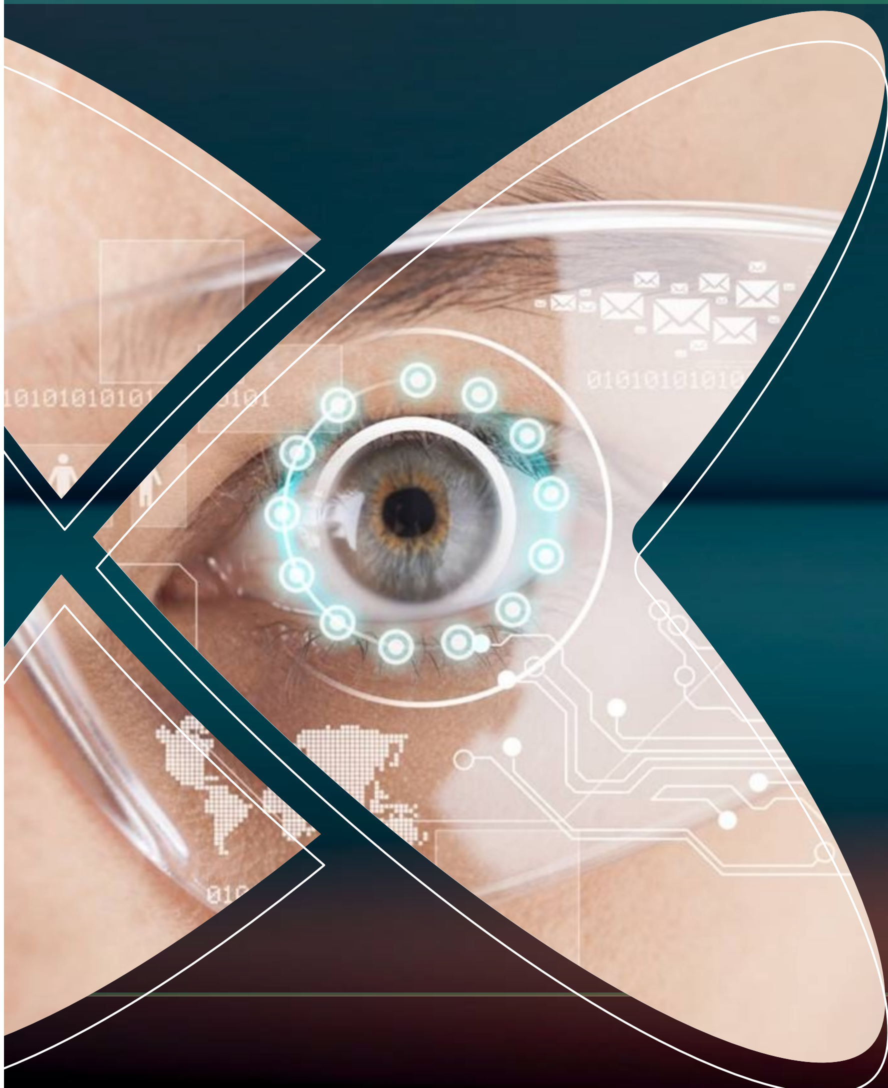
R.R. Naik *et al.*, *npj Computational Materials* **8**, 72 (2022)
https://doi.org/10.1038/s41524-022-00751-5

Open Science



After sharing our environmental chamber design with two other labs, we're open sourcing the entire "generative design" of hardware models: Bills of materials, assembly instructions, GitHub code, and manuscript.

Publication forthcoming…



Several of the co-authors of the papers you've just seen formed Xinterra, a startup dedicated to accelerating the development of new materials for sustainability. Co-founder Kedar Hippalgaonkar will share an update at the Acceleration Consortium meeting in Toronto Aug 30 – Sept 2, 2022.

xinterra

A New World of Materials

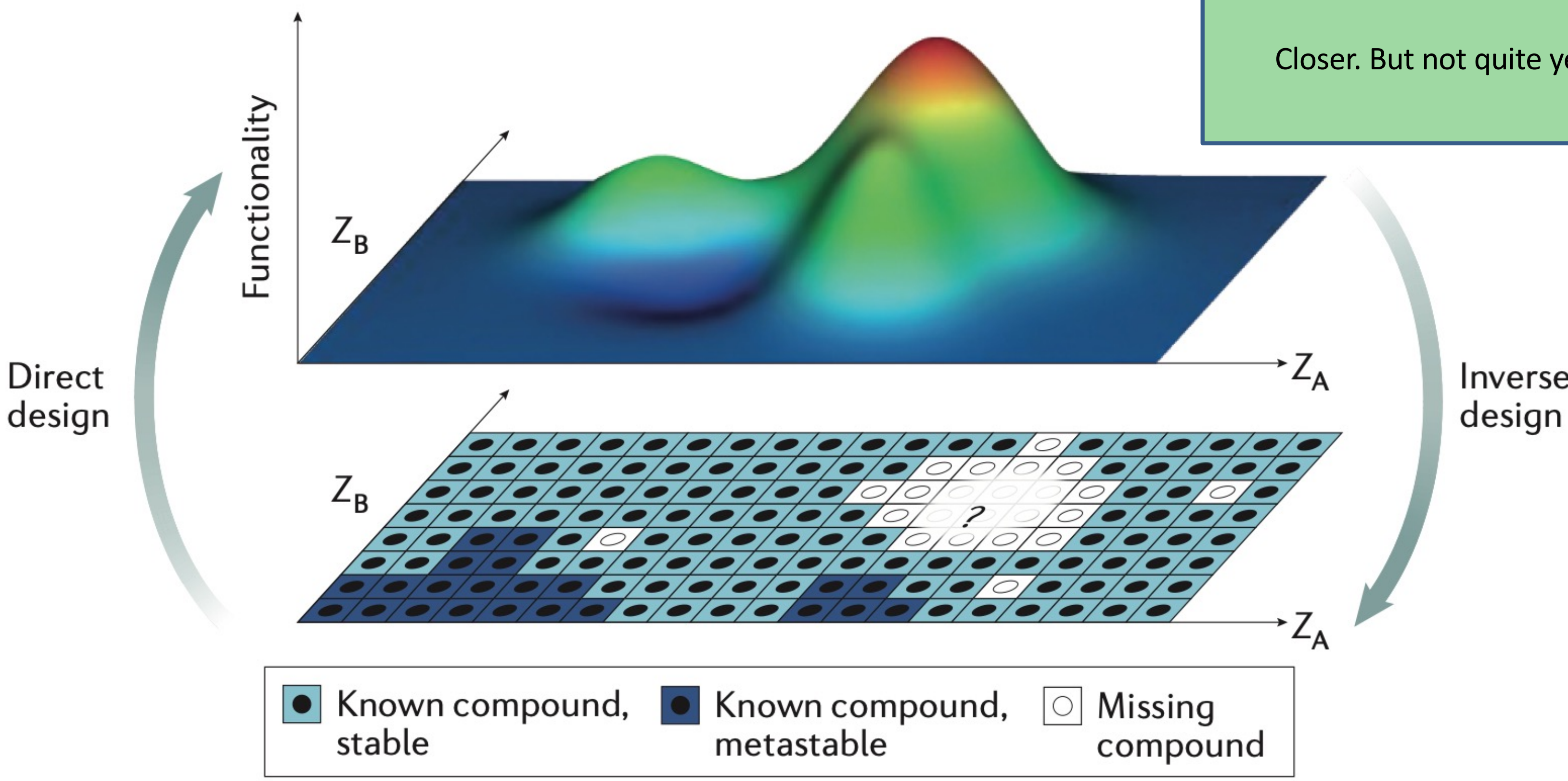
Faster and efficient materials development

Accelerated Materials Laboratory for Sustainability

Inverse Design: Are We There Yet?

So, are we there yet?

Closer. But not quite yet.



A. Zunger, *Nat. Rev. Chem.* **2**, 121 (2018)
https://doi.org/10.1038/s41570-018-0121

“Green Spaces” in Inverse Design

- Materials representations that unlock simpler algorithms
- Improved “refinements” to existing models
- Transformers
- Synthesizability estimators
- Knowledge inference & uncertainty estimation
- Ethics & Dual Use

Here are some promising research areas.

Lab Logo: "A leaf blended with an integrated circuit"

Hugging Face
DALL·E mini by craiyon.com

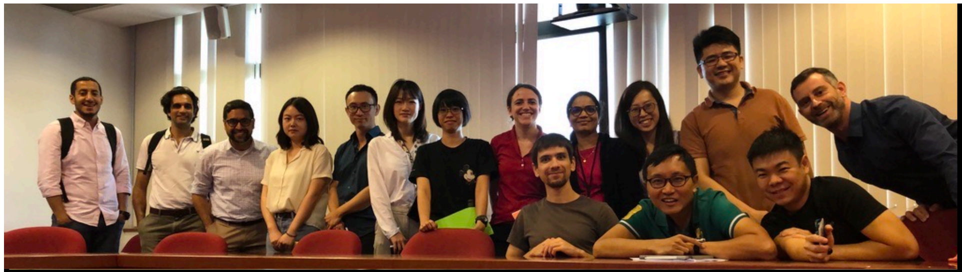
…I think with the right use cases, they can be transformative. We used this to inspire our new lab logo. We then passed these inspirations to a professional logo designer, and got…

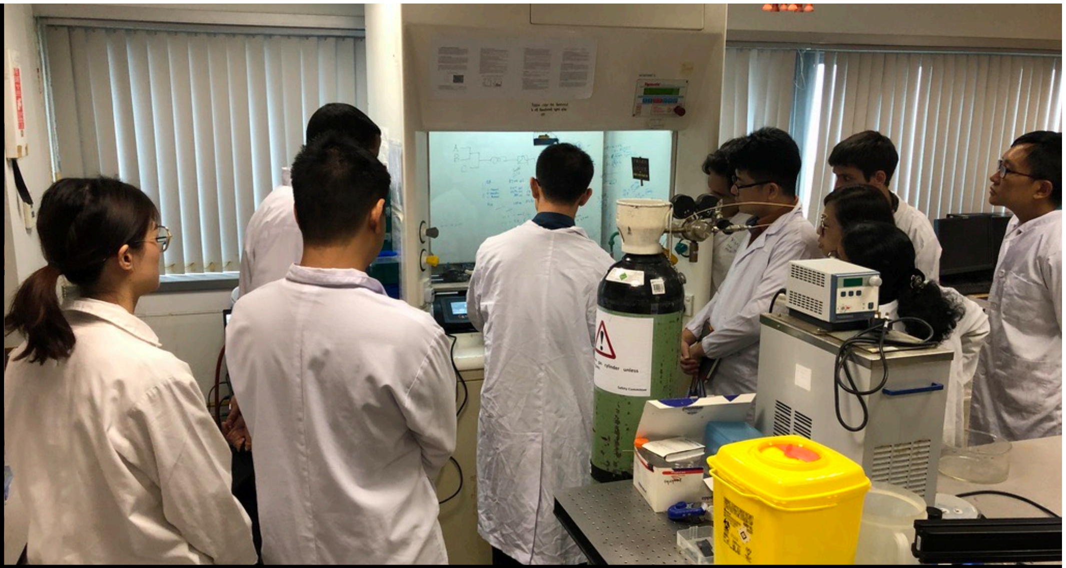
Lab Logo: “A leaf blended with an integrated circuit”

Arjie Lupac,
entrepreneur

Accelerated
Materials
Laboratory for
Sustainability

…this. I think combining human and machine intelligence might still be the way to go in this field for some time.





Here's an acknowledgement to some of the humans who made these past years enjoyable and successful.


Here’s an acknowledgement to some of the humans who made these past years enjoyable and successful.

Goal:

You give me a set of properties,
I give you a material.

We're not there yet, but we've made progress.

Perhaps you can help make this possible.

Use your power, responsibly.


Photo by http://www.zainalandzainal.com/

https://twitter.com/toniobuonassisi

https://www.LinkedIn.com/today/author/tonio-buonassisi-7854543

https://pv-lab.github.io/perovskit/