DOI: 10.5281/zenodo.5604052

# Getting to the Future Faster: the FAIR Trade

*Spoiler Alert: It's not just about the data!*


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CDO, PARADIM Materials Innovation Platform

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| The FAIR Guiding Principles | |
|---|---|
| **Findable:** | |
| F1 | Data and metadata are assigned a globally unique and persistent identifier |
| F2 | Data are described with rich metadata (defined by R1 below) |
| F3 | Metadata clearly and explicitly include the identifier of the data it describes |
| F4 | Data and metadata are registered or indexed in a searchable resource |
| **Accessible:** | |
| A1 | Data and metadata are retrievable by their identifier using a standardized communications protocol |
| A1.1 | The protocol is open, free, and universally implementable |
| A1.2 | The protocol allows for an authentication and authorization procedure, where necessary |
| A2 | Metadata are accessible, even when the data are no longer available |
| **Interoperable:** | |
| I1 | Data and metadata use a formal, accessible, shared, and broadly applicable language for knowledge representation. |
| I2 | Data and metadata use vocabularies that follow FAIR principles |
| I3 | Data and metadata include qualified references to other (meta)data |
| **Reusable:** | |
| R1 | Data and metadata are richly described with a plurality of accurate and relevant attributes |
| R1.1 | Data and metdata are released with a clear and accessible data usage license |
| R1.2 | Data and metadata are associated with detailed provenance |
| R1.3 | Data and metadata meet domain-relevant community standards |

Adapted from Wilkinson et al., 2016
https://fairtoolkit.pistoiaalliance.org/fair-guiding-principles/

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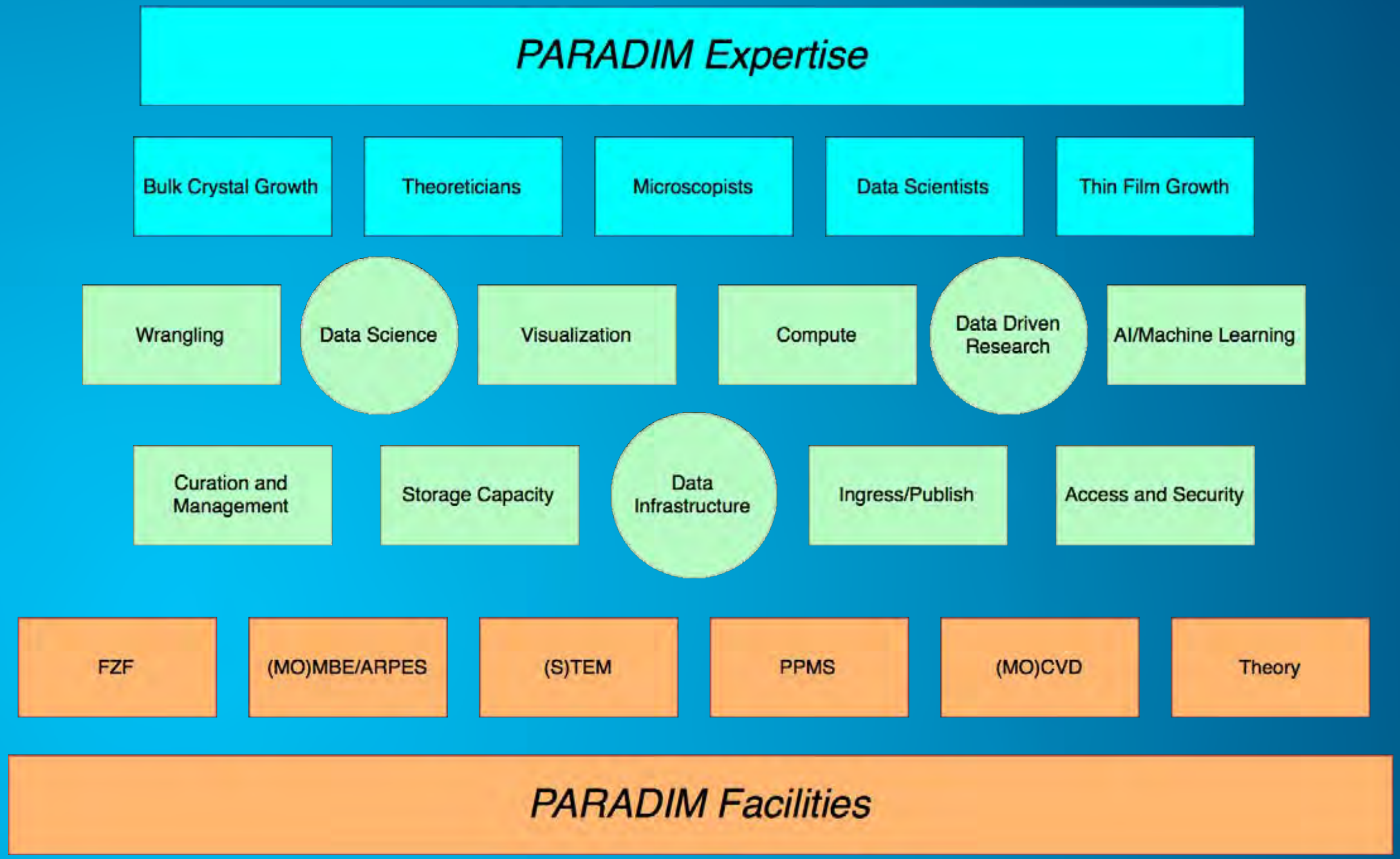
# PARADIM

User Facility:

- Crystal Growth Facility (Hopkins)
- PPMS and Characterization (Hopkins)
- Thin Film Deposition (Cornell)
- Electron Microscopy (Cornell)
- Theory/Modeling (Cornell/Clark Atlanta)

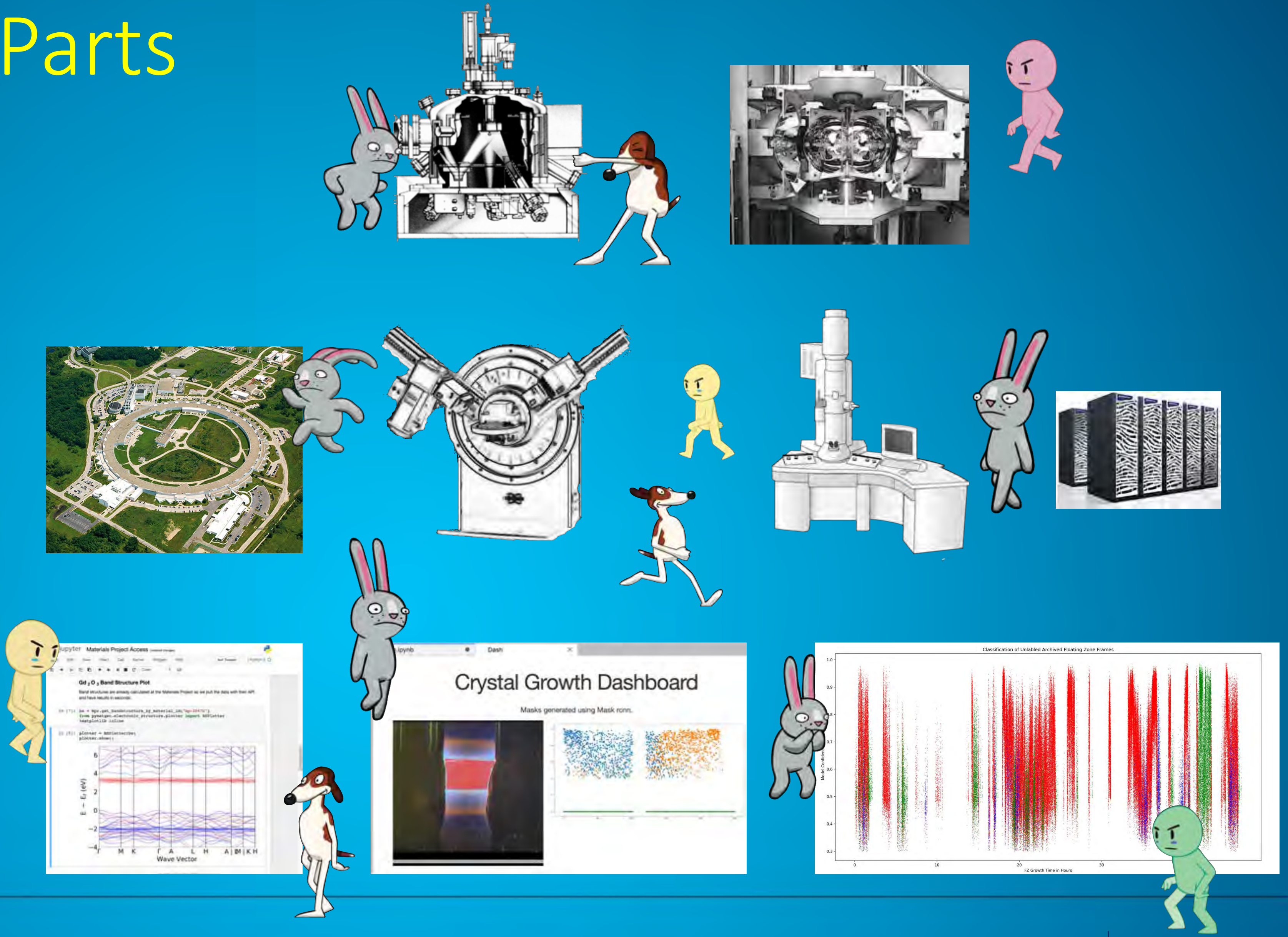
Data Challenges:

- User access/Security/Privacy
- Large Volume/Dispersed Activity
- Scalable visualization/analysis
- Education for broad user base
- Changing/Evolving infrastructure
- Time value of data



# Many Moving Parts

- Equipment
- People
- Ideas

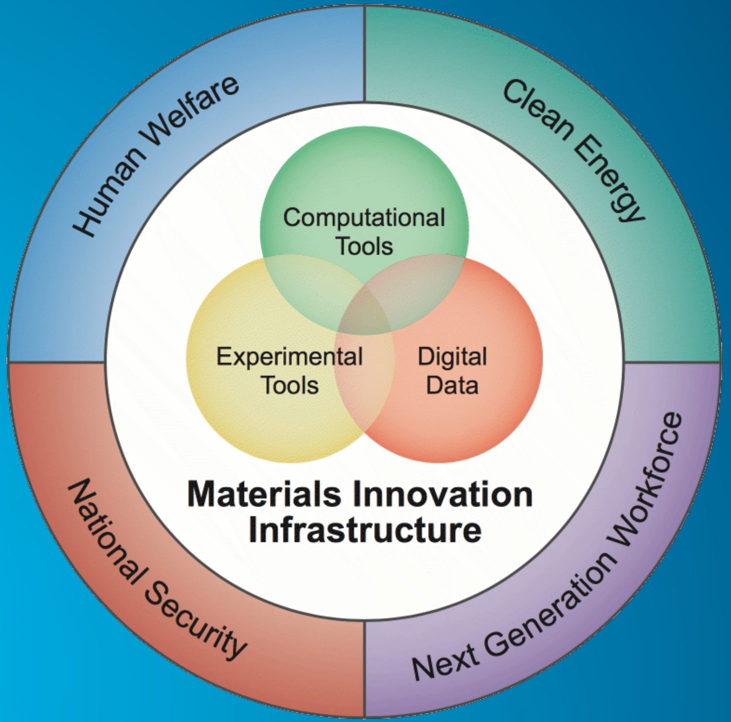


# Materials Genome Initiative (MGI)

## -*Discover, Develop, and Deploy Twice as Fast*

Strategic Goals:

- Facilitate Access to Materials Data
- Equip the Next-Generation Materials Workforce
- Integrate Experiments, Computation, and Theory
- Enable a Paradigm Shift in Materials Development

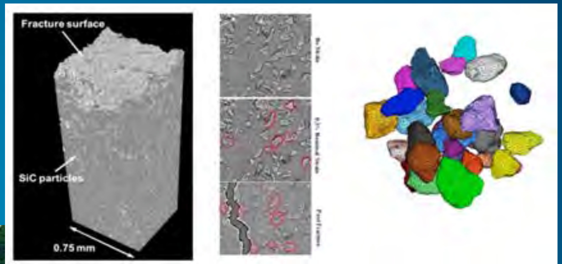



Cross Cutting Themes:

- Incentivizing open data and access of tools
- Structuring public-private partnerships
- Driving innovation across computation, data informatics, and experimentation
- Moving the community to a different cultural norm

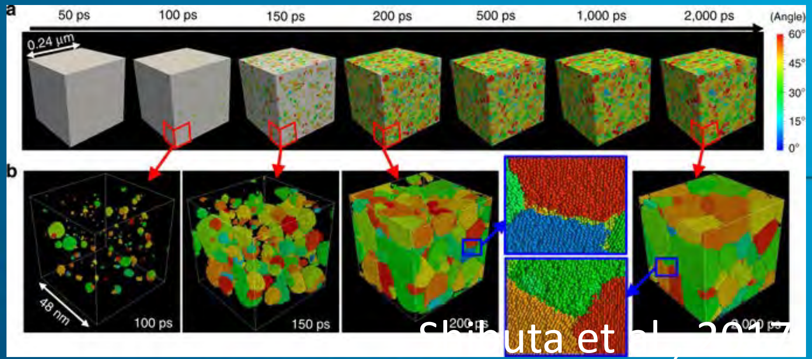
Refs: https://www.mgi.gov/content/mgi-infographic and https://www.mgi.gov/sites/default/files/documents/wadia_mgi_talk.pdf

De Carlo et al., 2012

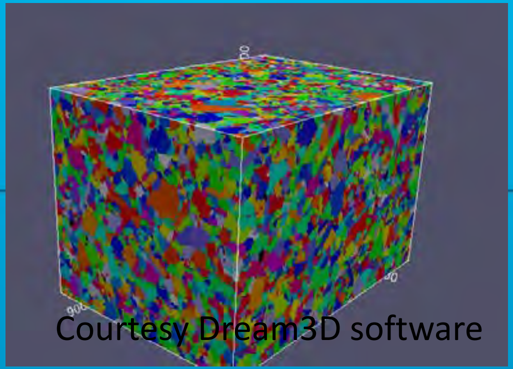



# Materials Data is Exploding

- Higher resolution
- Shorter time scales
- Higher dimensionality
- Dynamic experiments
- Larger simulations
- Tighter processing control




Shibuta et al., 2017

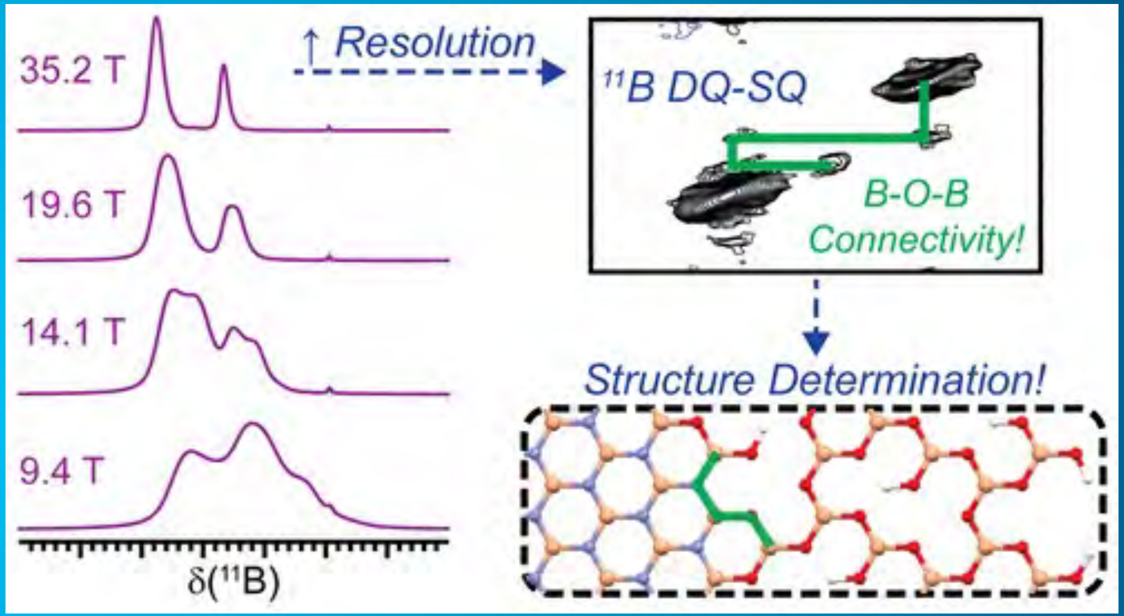


Courtesy Dream3D software

# What's the Value of Data?

*Superior Resolution Solves Structure Dilemma*

- Oxidative Dehydrogenation Catalyst
- $^{11}$B with $B_0$ = 35.2 T
- Superior resolution
- Distinguish active B species
- Determine the critical structure




Dorn et al, 2021 ACS DOI 10.1021/acscatal.0c03762

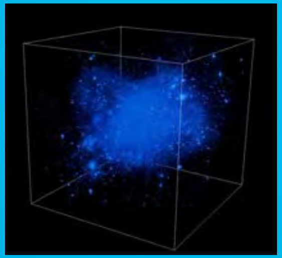
# Disruptive Change

**1000 Years:** empirical descriptions of natural phenomena

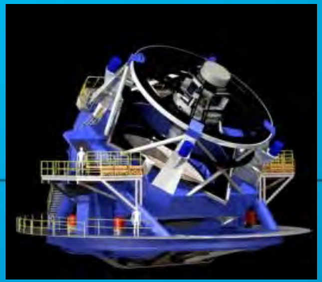
**100's Years:** theoretical branch using models, generalizations

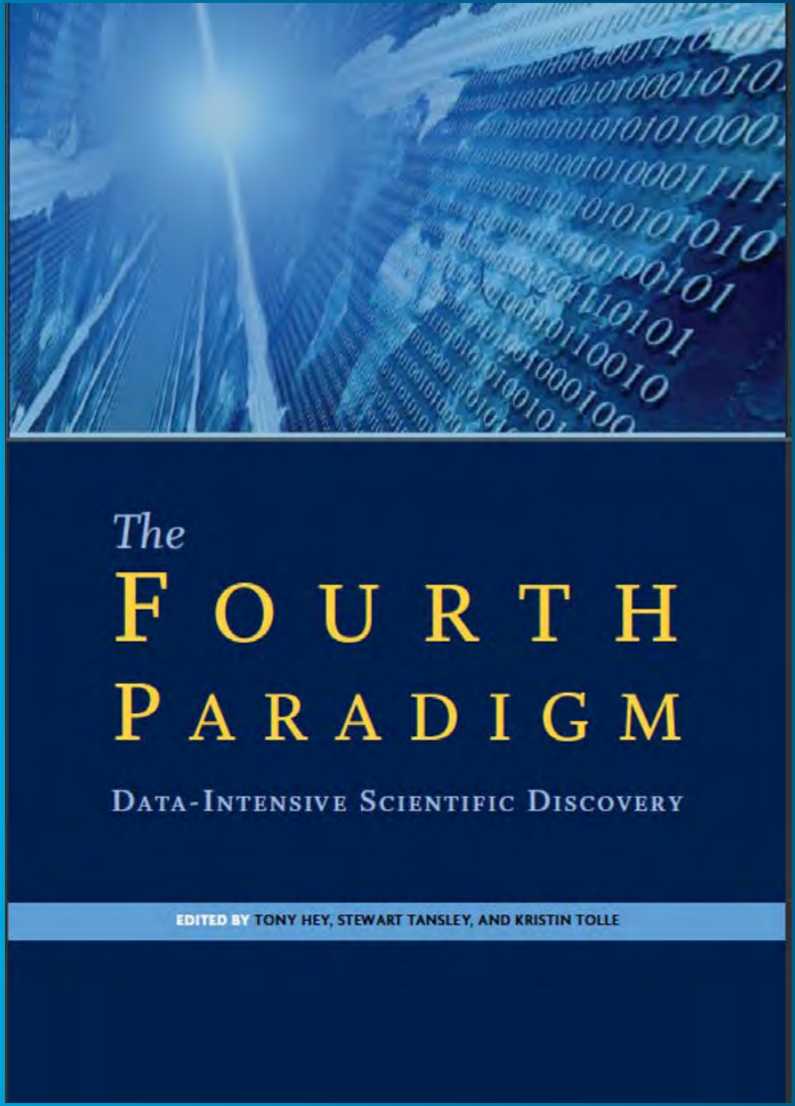
$$\left(\frac{\dot{a}}{a}\right)^2 = \frac{4\pi G\rho}{3} - \mathrm{K}\frac{c^2}{a^2}$$

**10's Years:** computational branch simulation of complex phenomena



**Now:** data intensive science, discovery directly from the data. Synthesizes theory, experiment and computation with statistics

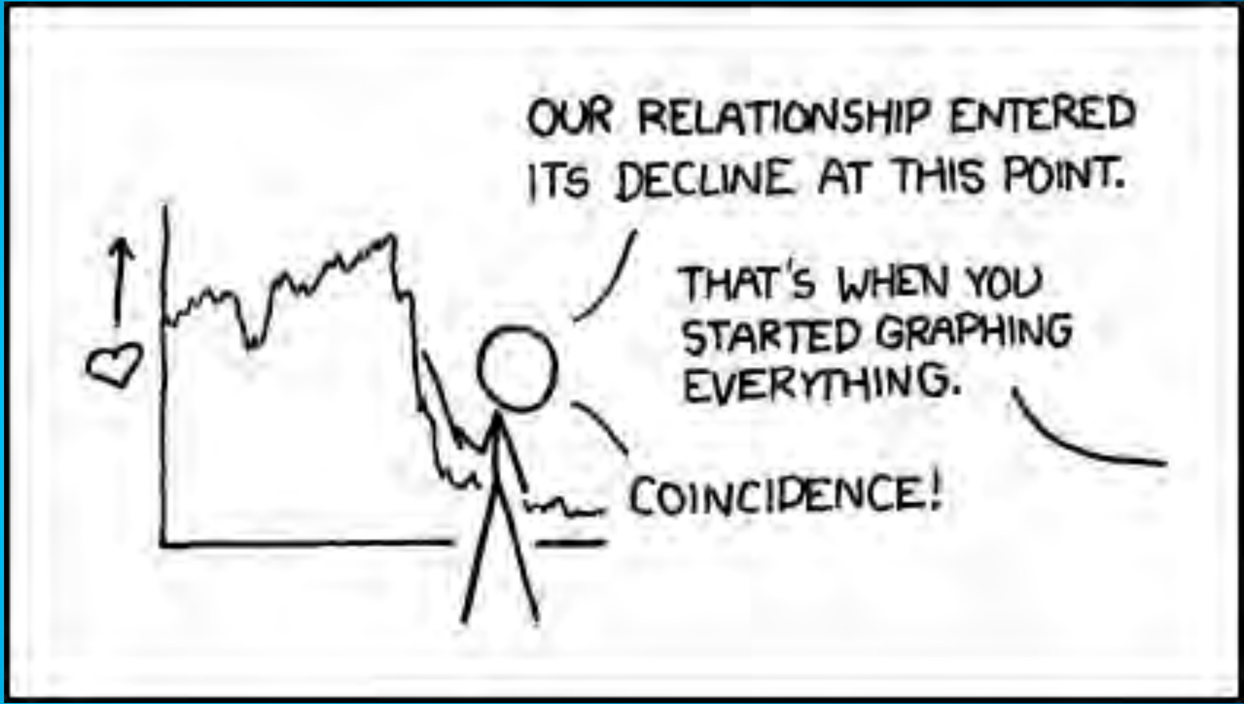




# What's the Value of Data?

*Provides Proof of What We Assert – the Heart of Scientific Knowledge*

- Property measurements
- Probes structures and processes
- Prove/Eliminate hypotheses
- Enable validation




https://xkcd.com/523

# What’s the Cost of Data?

*Data is Dearly Won!*

- Instrumentation
- Scientist Time
- Expertise
- Validation

- Curation
  - Annotation
  - Storage
  - Maintenance

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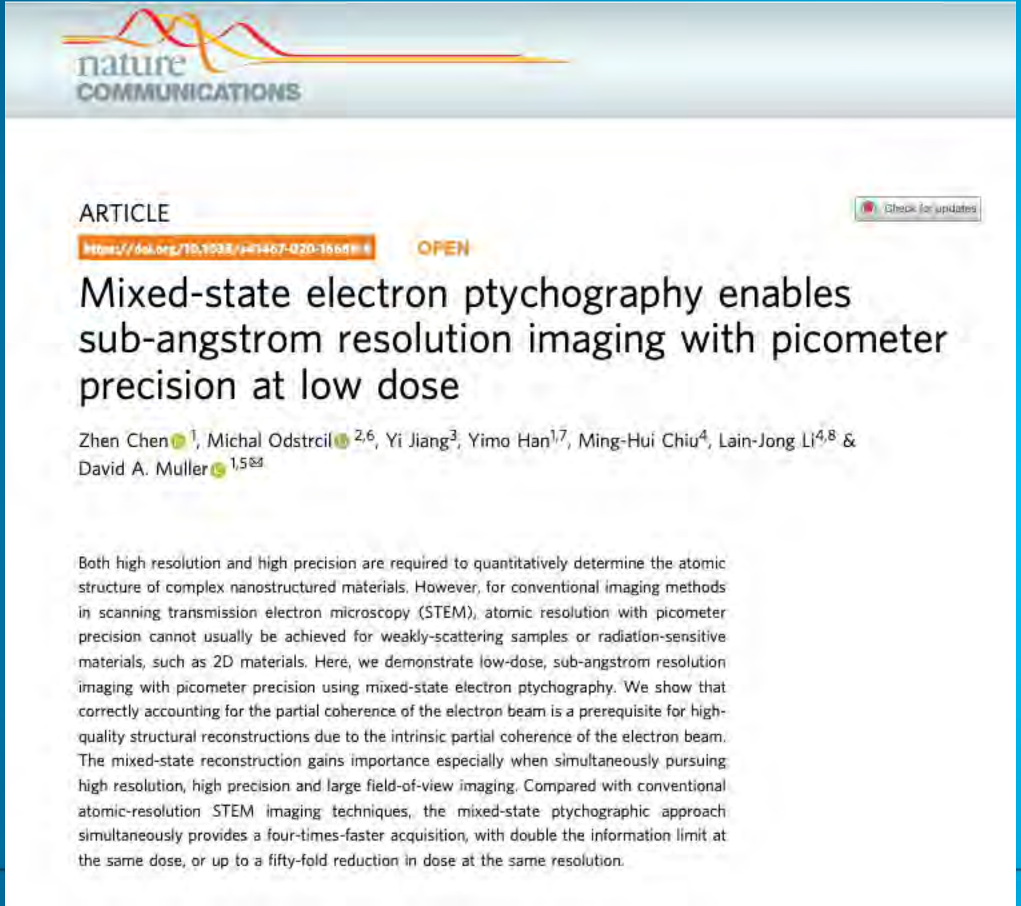
# The Value of Data Changes Over Time

*Data regains value over time if it can be reused*



nature COMMUNICATIONS

ARTICLE

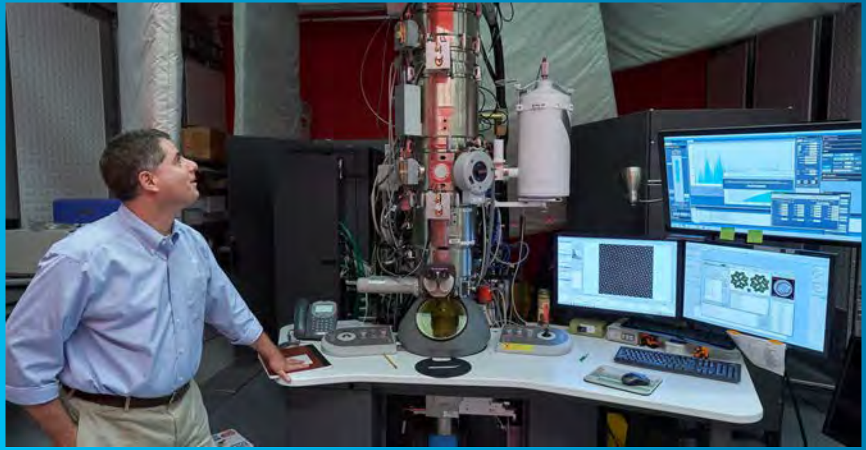
Check for updates

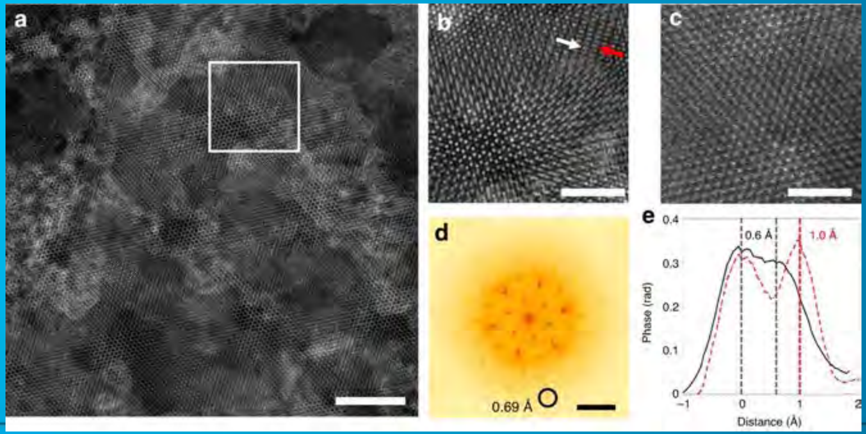
https://doi.org/10.1038/s41467-020-16688-6 OPEN

## Mixed-state electron ptychography enables sub-angstrom resolution imaging with picometer precision at low dose

Zhen Chen[1], Michal Odstrcil[2,6], Yi Jiang[3], Yimo Han[1,7], Ming-Hui Chiu[4], Lain-Jong Li[4,8] & David A. Muller[1,5]✉

Both high resolution and high precision are required to quantitatively determine the atomic structure of complex nanostructured materials. However, for conventional imaging methods in scanning transmission electron microscopy (STEM), atomic resolution with picometer precision cannot usually be achieved for weakly-scattering samples or radiation-sensitive materials, such as 2D materials. Here, we demonstrate low-dose, sub-angstrom resolution imaging with picometer precision using mixed-state electron ptychography. We show that correctly accounting for the partial coherence of the electron beam is a prerequisite for high-quality structural reconstructions due to the intrinsic partial coherence of the electron beam. The mixed-state reconstruction gains importance especially when simultaneously pursuing high resolution, high precision and large field-of-view imaging. Compared with conventional atomic-resolution STEM imaging techniques, the mixed-state ptychographic approach simultaneously provides a four-times-faster acquisition, with double the information limit at the same dose, or up to a fifty-fold reduction in dose at the same resolution.






Chen et al, Nature Comm, 2020, 10.1038/s41467-020-16688-6

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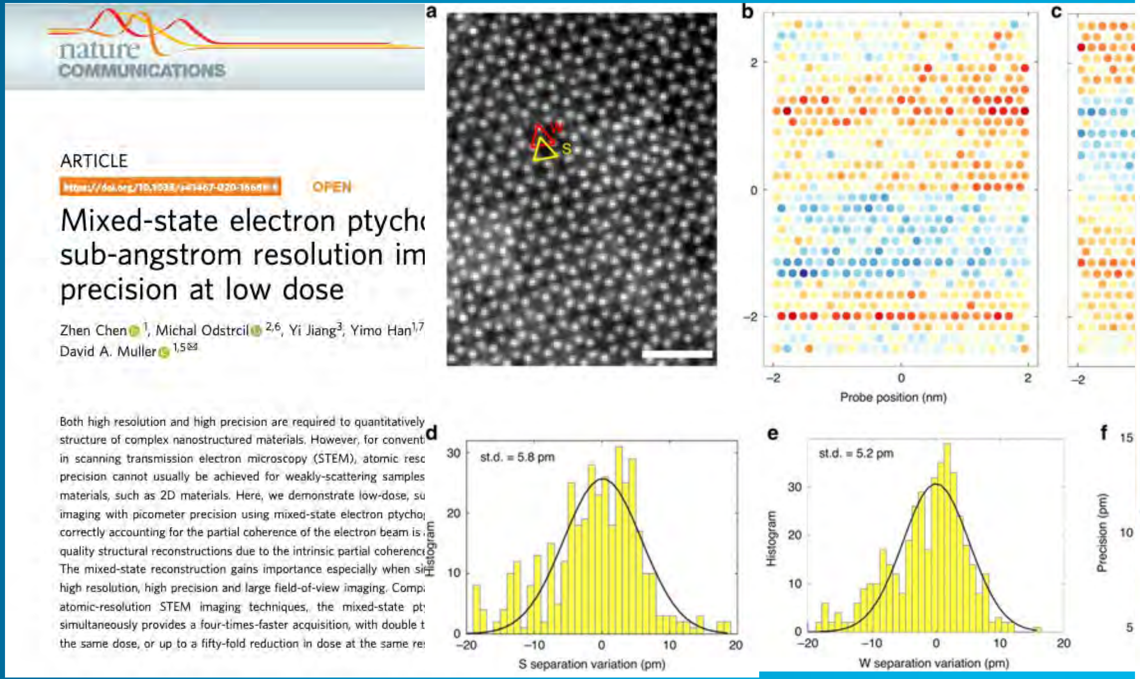


**Data set: Mixed-state electron ptychography enables sub-angstrom resolution imaging with picometer precision at low dose**

Zhen Chen, Michal Odstrcil, Yi Jiang, Yimo Han, Ming-Hui Chiu, Lain-Jong Li, David A. Muller

| Item | Link |
|---|---|
| Input Data (Matlab mat) | rawdata_1x_crop.mat |
| Output Result (png) | pty_crop_phase.png |
| Analysis Code 1 | https://github.com/muller-group-cornell/ptychography |
| Analysis Code 2 | https://www.psi.ch/en/sls/csaxs |

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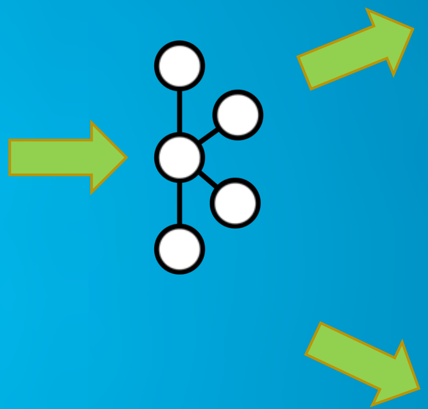
http//doi.org/10.34863/g4wa-0j57

# Seamless to User

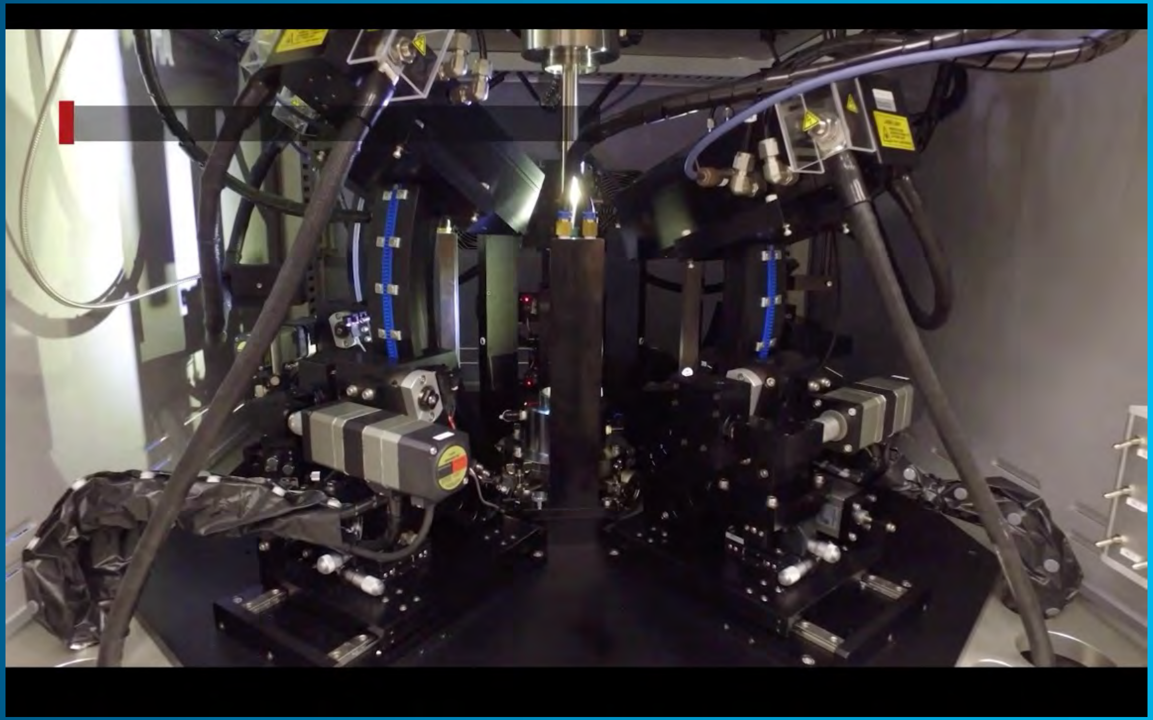
*Data regains value over time if it can be reused*

- Streaming Data
- Asynchronous
- Loosely Coupled
- Header metadata to DB
- PID



# Data Reuse Can Bring Unexpected Value

*Data regains value over time if it can be reused*

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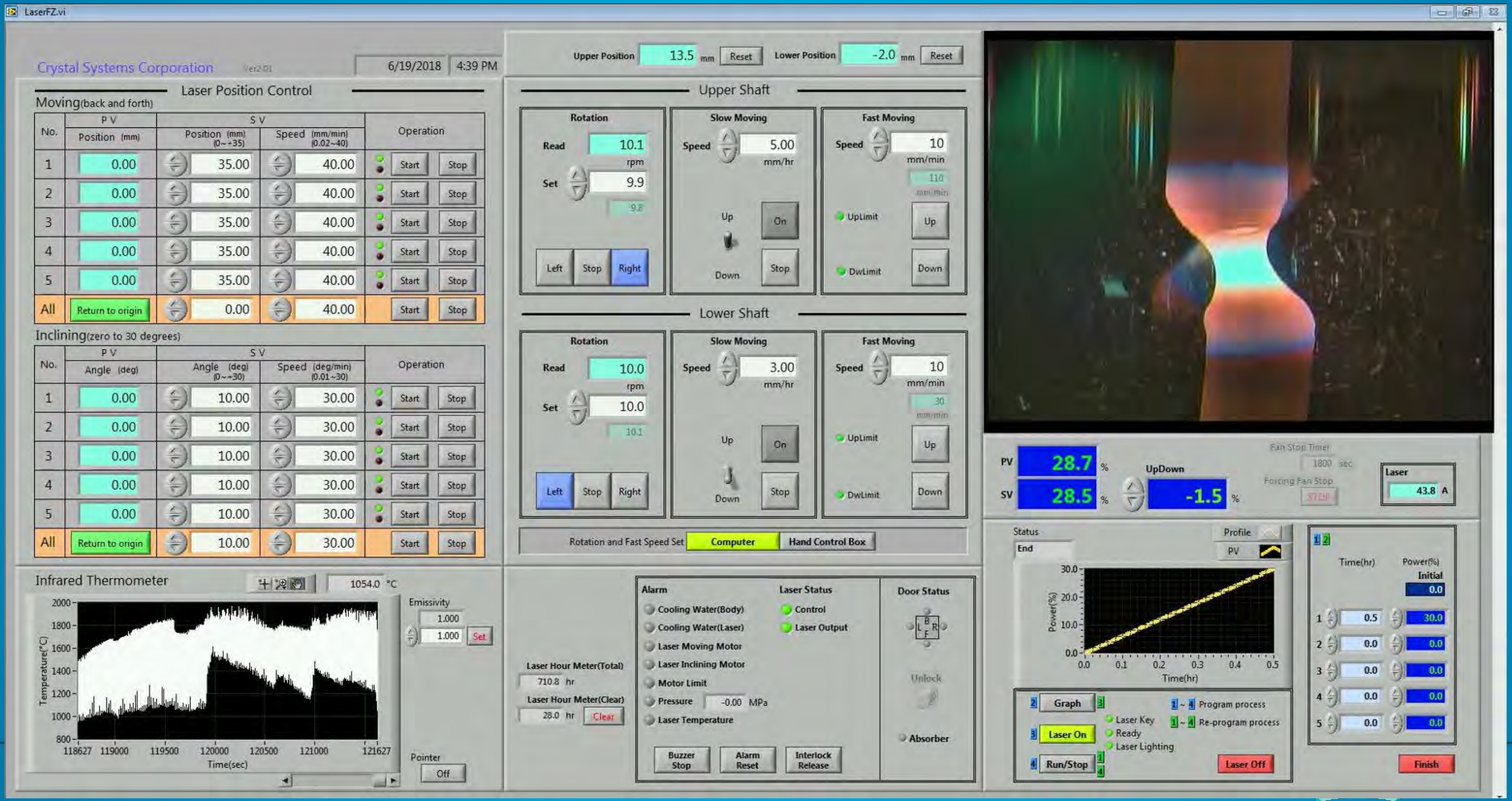


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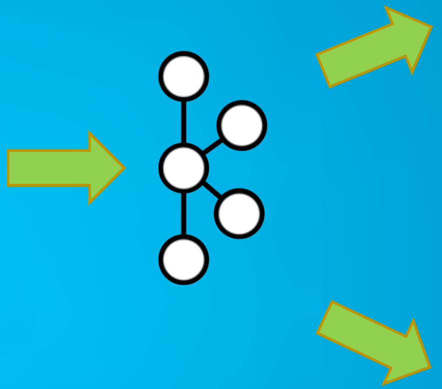

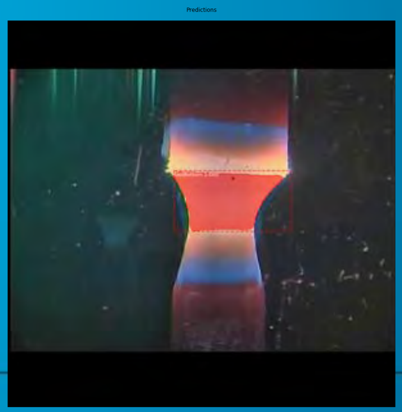

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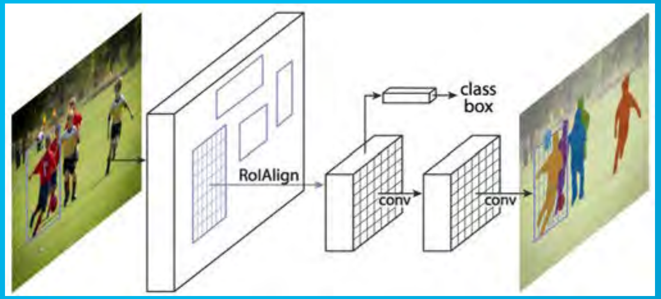
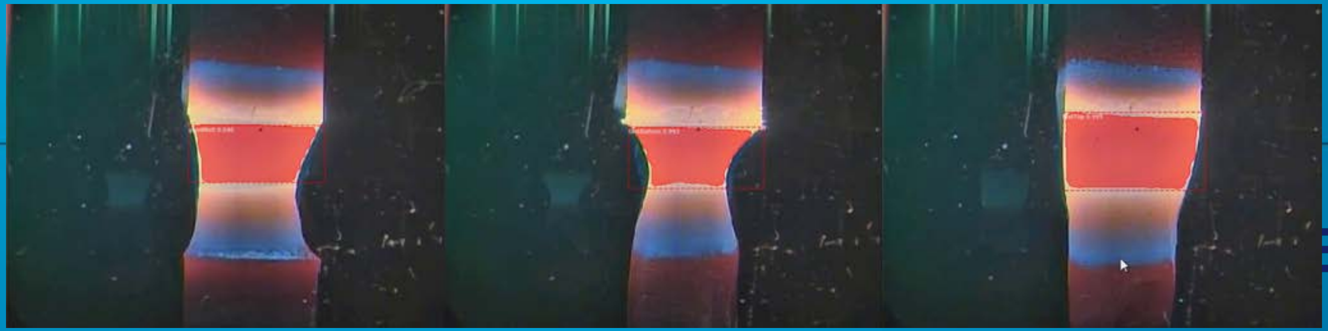
Mask R-CNN

He et al, 2017



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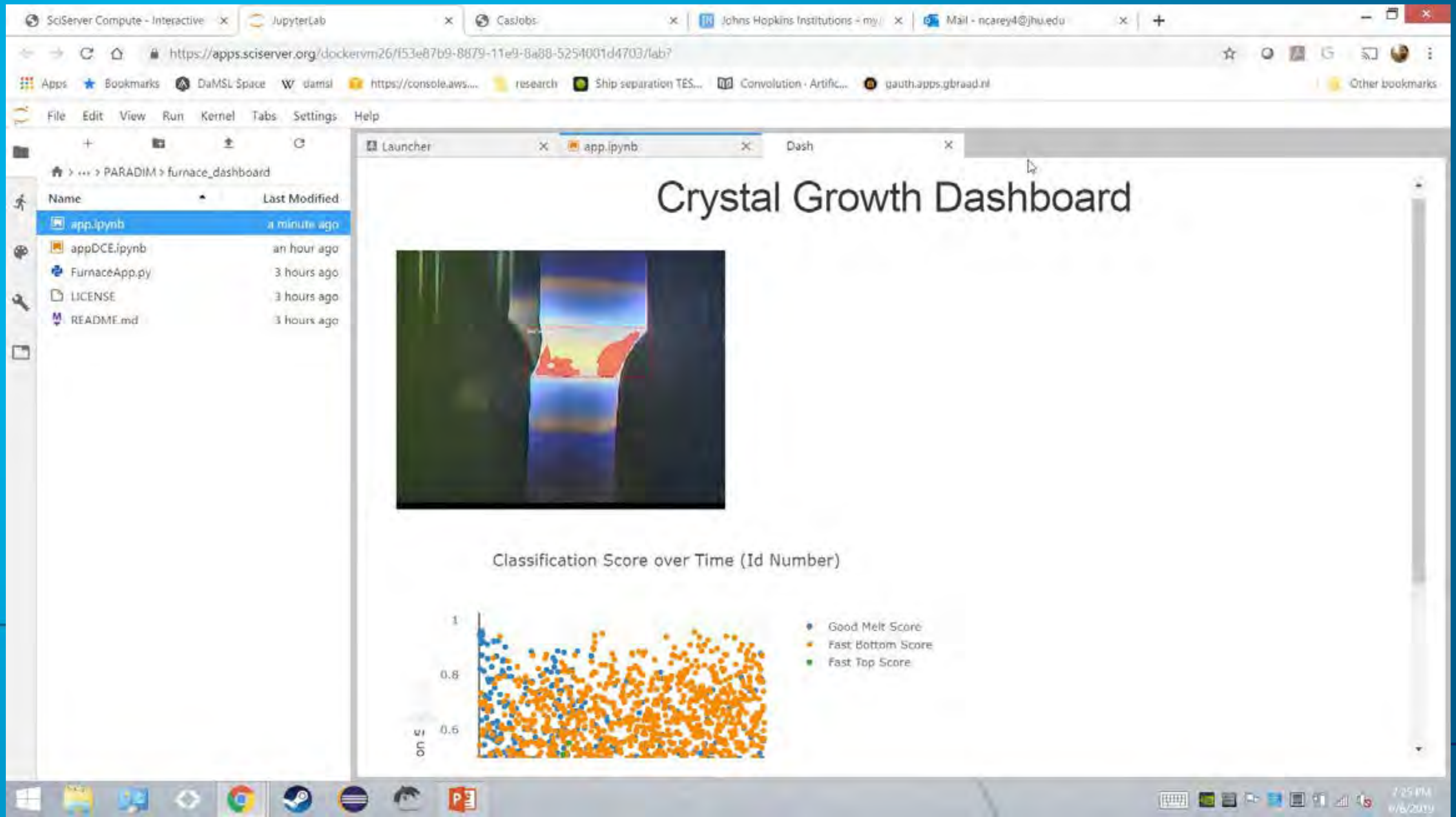
# Data Reuse in Real Time Deployment

*Data regains value over time if it can be reused*

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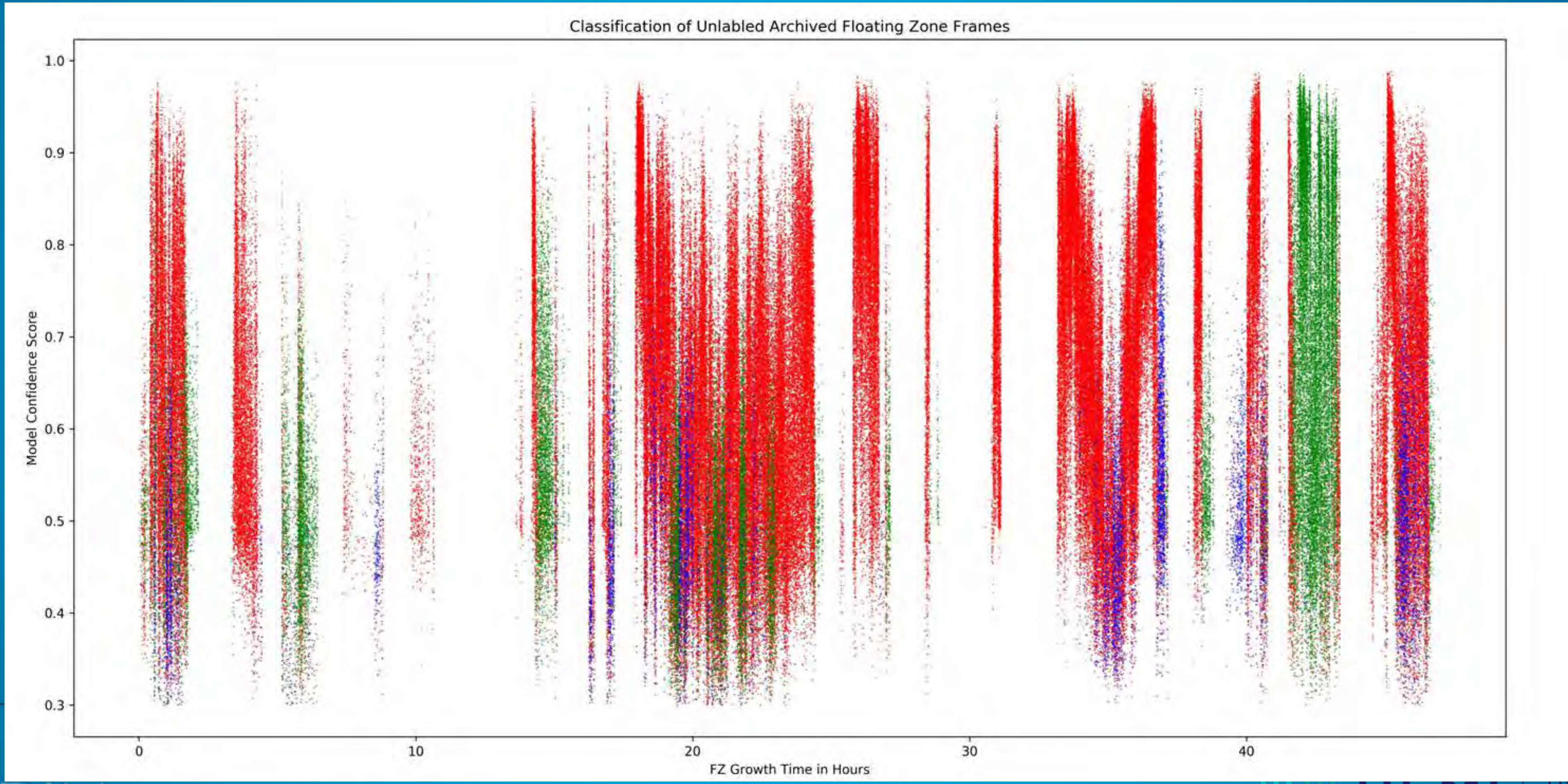


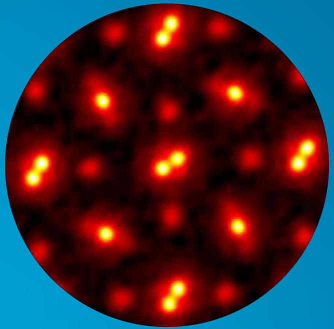
# Power, Practice, Leadership

- FAIR is a critical enabler of the MGI
  the currency of Materials Data Infrastructure


TMS 2017 Study
https://doi.org/10.7449/mdistudy_1

# Power, Practice, Leadership

- PARADIM is strategic for FAIR production
  - center of data production
  - microcosm of domain
  - many users
  - embedded training
  - in-house program



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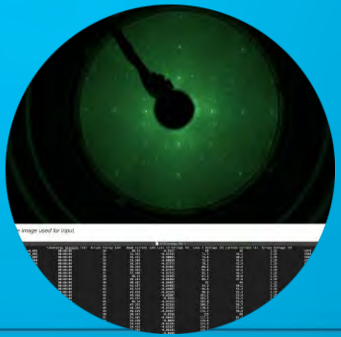
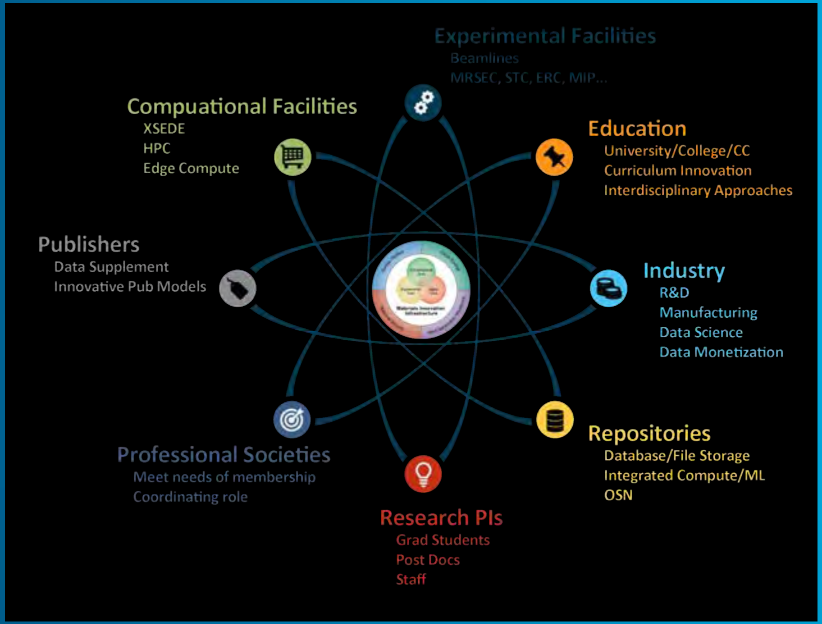


# Power, Practice, Leadership

- FAIR needs community





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# FAIR-ification: All Data is not Equal

**PARADIM Data Domains:**

- **physical samples** – digital twin/digital thread
- **synthesis recipes** – intent and realization
- **characterization** – structure and properties
- **codes/methods** – software, notebooks, infrastructure
- **reports** – publications and presentations
- **training materials** – lectures, problems, infrastructure

FAIR is a set of principles, but in practice depends on the type of data and the needs or desires of those sharing the data.

# FAIR Today Fairer Tomorrow

F: Searchable Metadata
- DataCite Search
- Google Data Search (schema.org)
- Web/Pub Links
- Digital Object Id (DOI)

A: DataCite API
- Year Embargo
- Individual Files

I: Community Standards
- File Formats
- Open Tools

R: License and Relevant Metadata
- CC-4.0-BY-NC-ND
- in development

| FAIR principle | FAIR Maturity Indicator |
|---|---|
| F1 | Data and metadata identifiers are unique and persistent |
| F2 | Metadata are structured (weak) or grounded in shared vocabularies (strong) |
| F3 | Data and metadata identifiers are included explicitly in metadata |
| F4 | Searchable in web-based search engines |
| A1.1 | Uses open free protocol for data & metadata retrieval |
| A1.2 | Data and metadata authentication and authorization |
| A2 | Metadata persistence |
| I1 | Data and metadata knowledge representation language (weak or strong) |
| I2 | Metadata uses FAIR vocabularies or ontologies (weak or strong) |
| I3 | Metadata contains qualified outward references |
| R1.1 | Metadata includes a license for data usage (weak or strong) |
| R1.2 | Metadata includes provenance (weak) |
| R1.3 | Metadata contains community standards (weak) |

weak - readable only by humans; strong - readable by machines

FAIR Data Maturity Model Specifications and Guidelines
https://doi.org/10.15497/rda00050

# FAIR Today Fairer Tomorrow

**F:** Searchable Metadata

- DataCite Search
- Google Data Search (schema.org)
- Web/Pub Links
- Digital Object Id (DOI)

**A:** DataCite API

- Landing Page
- Year Embargo
- Individual Files

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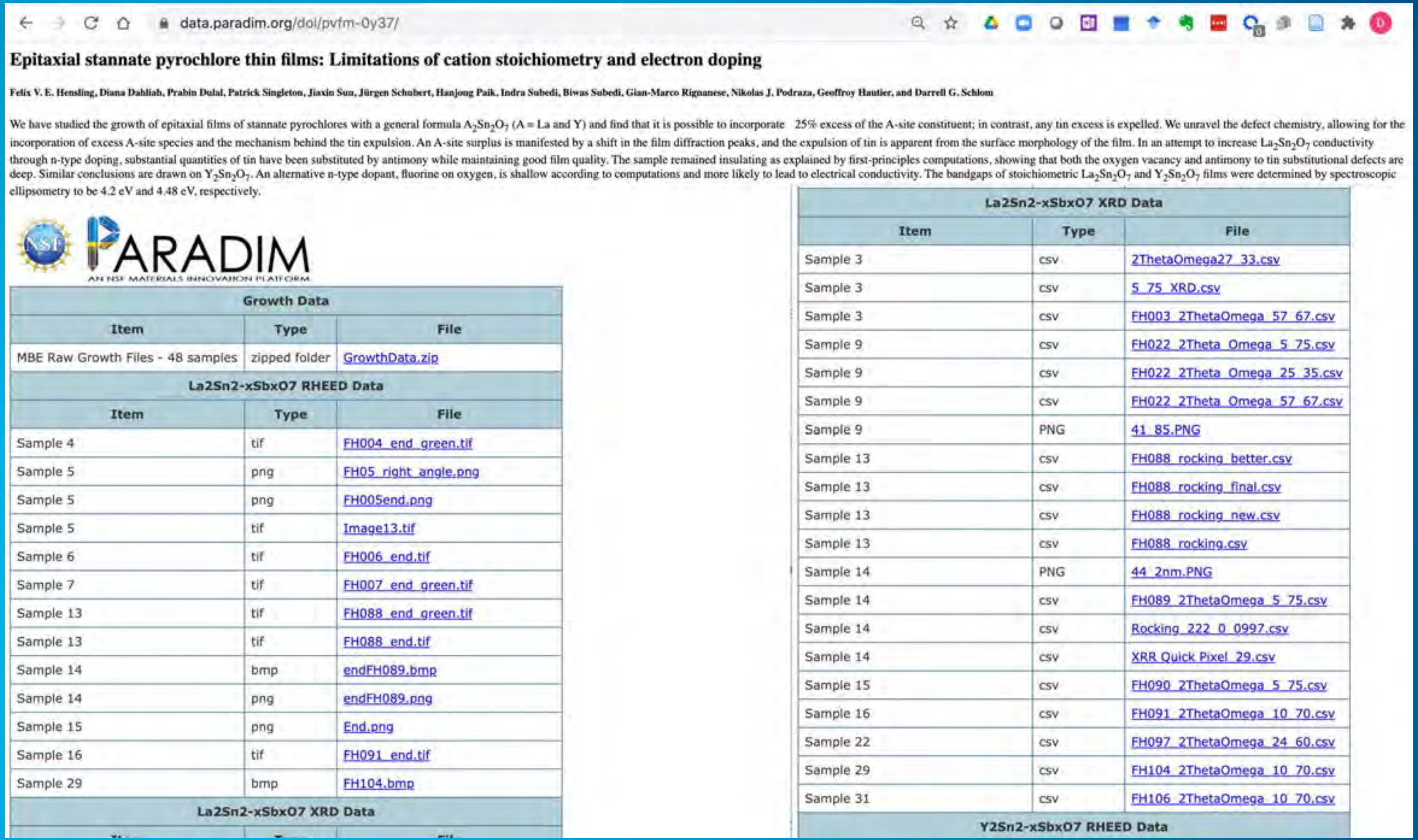
data.paradim.org/doi/pvfm-0y37/

**Epitaxial stannate pyrochlore thin films: Limitations of cation stoichiometry and electron doping**

Felix V. E. Hensling, Diana Dahliah, Prabin Dulal, Patrick Singleton, Jiaxin Sun, Jürgen Schubert, Hanjong Paik, Indra Subedi, Biwas Subedi, Gian-Marco Rignanese, Nikolas J. Podraza, Geoffroy Hautier, and Darrell G. Schlom

We have studied the growth of epitaxial films of stannate pyrochlores with a general formula $A_2Sn_2O_7$ (A = La and Y) and find that it is possible to incorporate 25% excess of the A-site constituent; in contrast, any tin excess is expelled. We unravel the defect chemistry, allowing for the incorporation of excess A-site species and the mechanism behind the tin expulsion. An A-site surplus is manifested by a shift in the film diffraction peaks, and the expulsion of tin is apparent from the surface morphology of the film. In an attempt to increase $La_2Sn_2O_7$ conductivity through n-type doping, substantial quantities of tin have been substituted by antimony while maintaining good film quality. The sample remained insulating as explained by first-principles computations, showing that both the oxygen vacancy and antimony to tin substitutional defects are deep. Similar conclusions are drawn on $Y_2Sn_2O_7$. An alternative n-type dopant, fluorine on oxygen, is shallow according to computations and more likely to lead to electrical conductivity. The bandgaps of stoichiometric $La_2Sn_2O_7$ and $Y_2Sn_2O_7$ films were determined by spectroscopic ellipsometry to be 4.2 eV and 4.48 eV, respectively.

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| Growth Data | | |
|---|---|---|
| Item | Type | File |
| MBE Raw Growth Files - 48 samples | zipped folder | GrowthData.zip |

| La2Sn2-xSbxO7 RHEED Data | | |
|---|---|---|
| Item | Type | File |
| Sample 4 | tif | FH004_end_green.tif |
| Sample 5 | png | FH05_right_angle.png |
| Sample 5 | png | FH005end.png |
| Sample 5 | tif | Image13.tif |
| Sample 6 | tif | FH006_end.tif |
| Sample 7 | tif | FH007_end_green.tif |
| Sample 13 | tif | FH088_end_green.tif |
| Sample 13 | tif | FH088_end.tif |
| Sample 14 | bmp | endFH089.bmp |
| Sample 14 | png | endFH089.png |
| Sample 15 | png | End.png |
| Sample 16 | tif | FH091_end.tif |
| Sample 29 | bmp | FH104.bmp |

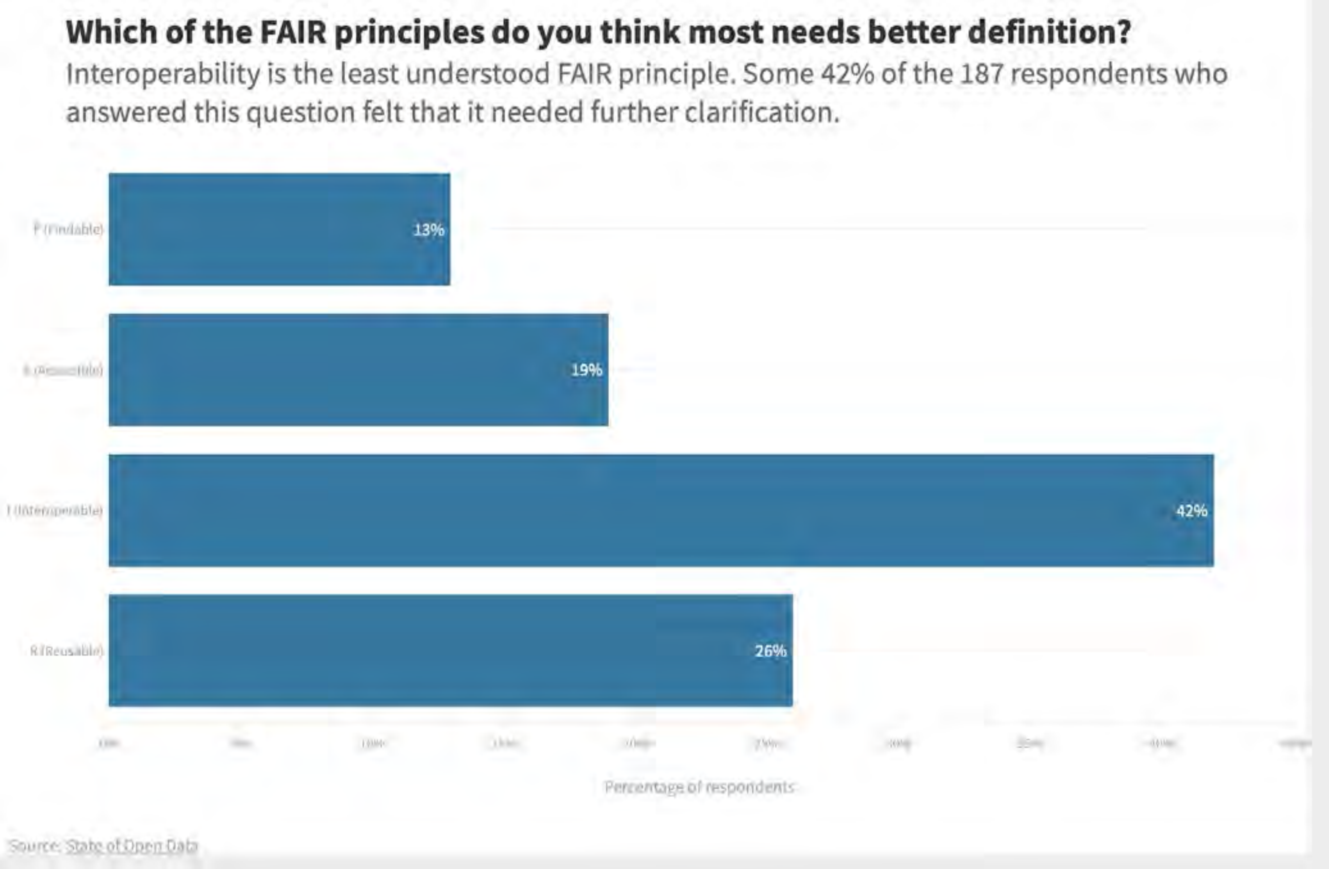
| La2Sn2-xSbxO7 XRD Data | | |
|---|---|---|
| Item | Type | File |
| Sample 3 | csv | 2ThetaOmega27_33.csv |
| Sample 3 | csv | 5_75_XRD.csv |
| Sample 3 | csv | FH003_2ThetaOmega_57_67.csv |
| Sample 9 | csv | FH022_2Theta_Omega_5_75.csv |
| Sample 9 | csv | FH022_2Theta_Omega_25_35.csv |
| Sample 9 | csv | FH022_2Theta_Omega_57_67.csv |
| Sample 9 | PNG | 41_85.PNG |
| Sample 13 | csv | FH088_rocking_better.csv |
| Sample 13 | csv | FH088_rocking_final.csv |
| Sample 13 | csv | FH088_rocking_new.csv |
| Sample 13 | csv | FH088_rocking.csv |
| Sample 14 | PNG | 44_2nm.PNG |
| Sample 14 | csv | FH089_2ThetaOmega_5_75.csv |
| Sample 14 | csv | Rocking_222_0_0997.csv |
| Sample 14 | csv | XRR_Quick_Pixel_29.csv |
| Sample 15 | csv | FH090_2ThetaOmega_5_75.csv |
| Sample 16 | csv | FH091_2ThetaOmega_10_70.csv |
| Sample 22 | csv | FH097_2ThetaOmega_24_60.csv |
| Sample 29 | csv | FH104_2ThetaOmega_10_70.csv |
| Sample 31 | csv | FH106_2ThetaOmega_10_70.csv |

Y2Sn2-xSbxO7 RHEED Data

# FAIR Today Fairer Tomorrow

I: Community Standards
- Standard File Formats
- Open Tools

R: License and Relevant Metadata
- CC-4.0-BY-NC-ND
- in development




source: State of Open Data

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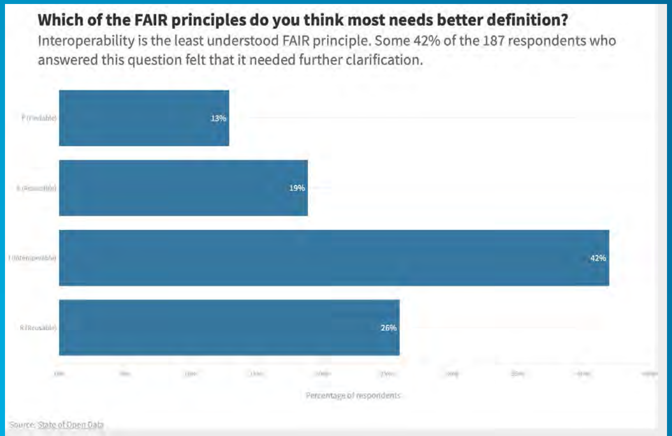


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# FAIR Today Fairer Tomorrow

1. Publication linked
   - Characterization
   - Reproducibility
   - Persistent Identifiers (DOI)
2. How do we improve?

**Dataset: Charge order textures induced by non-linear couplings in a half-doped manganite**

Dataset

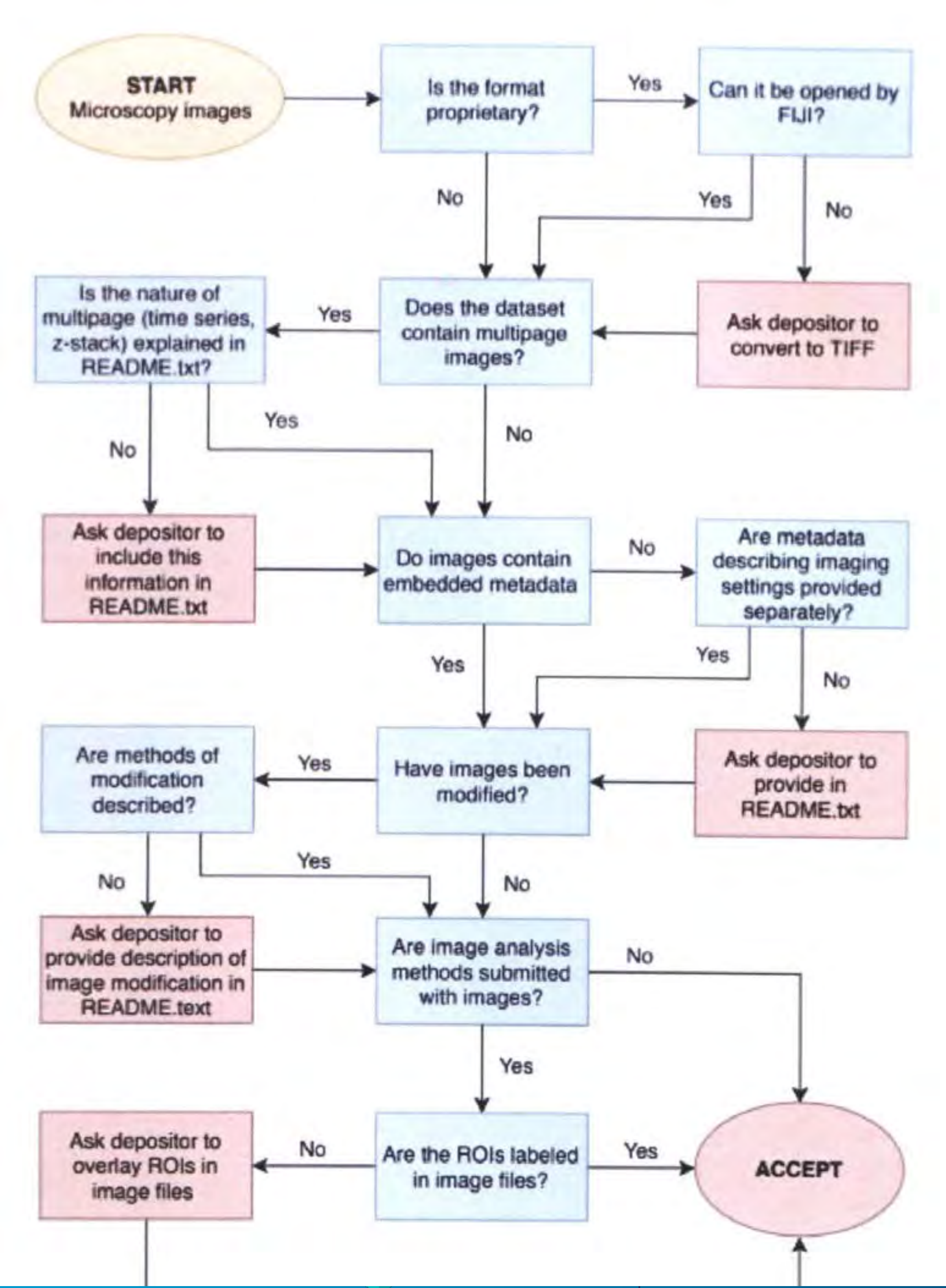
Ismail El Baggari, David Baek, Michael Zachman, Di Lu, Yasuyuki Hikita, Harold Hwang, Elizabeth Nowadnick & Lena Kourkoutis

Dataset published 2021 via PARADIM, an NSF Materials Innovation Platform

Raw data associated with publication. The self-organization of strongly interacting electrons into superlattice structures underlies the properties of many quantum materials. How these electrons arrange within the superlattice dictates what symmetries are broken and what ground states are stabilized. Here we show that cryogenic scanning transmission electron microscopy (cryo-STEM) enables direct mapping of local symmetries and order at the intra-unit-cell level in the model charge-ordered system Nd1/2Sr1/2MnO3. In addition to imaging the prototypical site-centered charge order, we discover the nanoscale coexistence of an exotic intermediate state which mixes site and bond order and breaks inversion symmetry. We further show that nonlinear coupling of distinct lattice modes controls the selection between competing ground states. The results demonstrate the importance of lattice coupling for understanding and manipulating the character of electronic self- organization and that cryo-STEM can reveal local order in strongly correlated systems at the atomic scale. keywords:

Created May 27, 2021, 21:22:23 UTC. Findable

https://doi.org/10.34863/bg5n-4s68

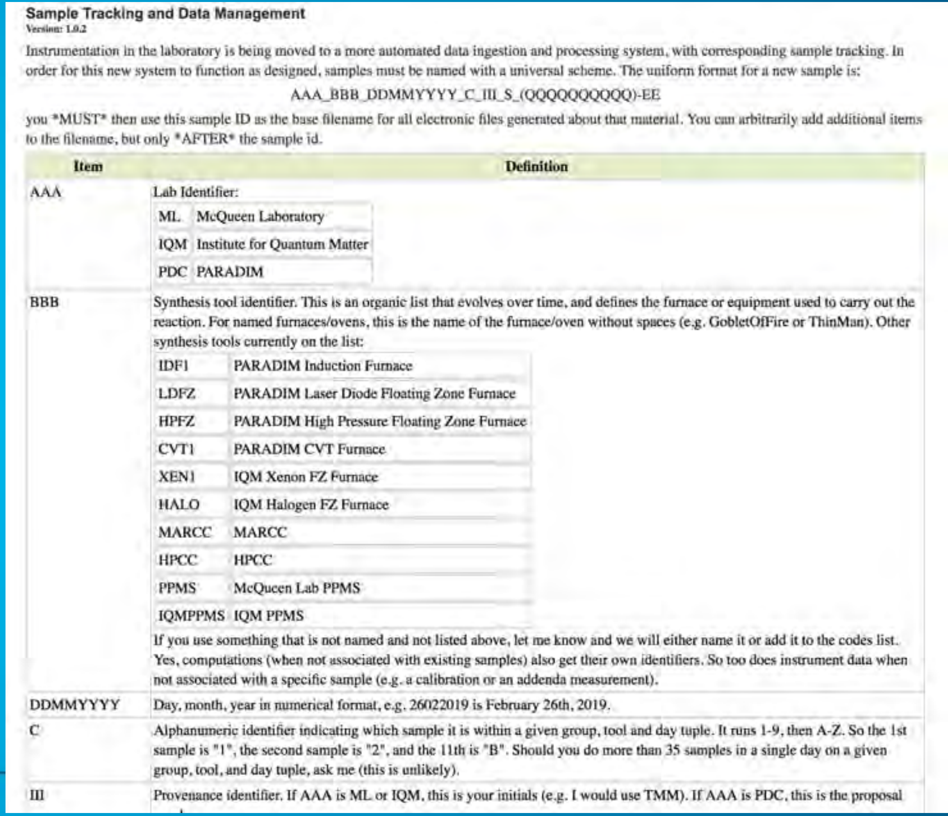



AN NSF MATERIALS INNOVATION PLATFORM

# FAIR Physical Samples

Digital Object Proxy

- digital twin
- digital thread
- entry point to re-creation

**Sample Tracking and Data Management**
Version: 1.0.2

Instrumentation in the laboratory is being moved to a more automated data ingestion and processing system, with corresponding sample tracking. In order for this new system to function as designed, samples must be named with a universal scheme. The uniform format for a new sample is:

AAA_BBB_DDMMYYYY_C_III_S_(QQQQQQQQQ)-EE

you *MUST* then use this sample ID as the base filename for all electronic files generated about that material. You can arbitrarily add additional items to the filename, but only *AFTER* the sample id.

| Item | Definition |
|---|---|
| AAA | Lab Identifier:<br>ML McQueen Laboratory<br>IQM Institute for Quantum Matter<br>PDC PARADIM |
| BBB | Synthesis tool identifier. This is an organic list that evolves over time, and defines the furnace or equipment used to carry out the reaction. For named furnaces/ovens, this is the name of the furnace/oven without spaces (e.g. GobletOfFire or ThinMan). Other synthesis tools currently on the list:<br>IDF1 PARADIM Induction Furnace<br>LDFZ PARADIM Laser Diode Floating Zone Furnace<br>HPFZ PARADIM High Pressure Floating Zone Furnace<br>CVT1 PARADIM CVT Furnace<br>XEN1 IQM Xenon FZ Furnace<br>HALO IQM Halogen FZ Furnace<br>MARCC MARCC<br>HPCC HPCC<br>PPMS McQueen Lab PPMS<br>IQMPPMS IQM PPMS<br>If you use something that is not named and not listed above, let me know and we will either name it or add it to the codes list. Yes, computations (when not associated with existing samples) also get their own identifiers. So too does instrument data when not associated with a specific sample (e.g. a calibration or an addenda measurement). |
| DDMMYYYY | Day, month, year in numerical format, e.g. 26022019 is February 26th, 2019. |
| C | Alphanumeric identifier indicating which sample it is within a given group, tool and day tuple. It runs 1-9, then A-Z. So the 1st sample is "1", the second sample is "2", and the 11th is "B". Should you do more than 35 samples in a single day on a given group, tool, and day tuple, ask me (this is unlikely). |
| III | Provenance identifier. If AAA is ML or IQM, this is your initials (e.g. I would use TMM). If AAA is PDC, this is the proposal |

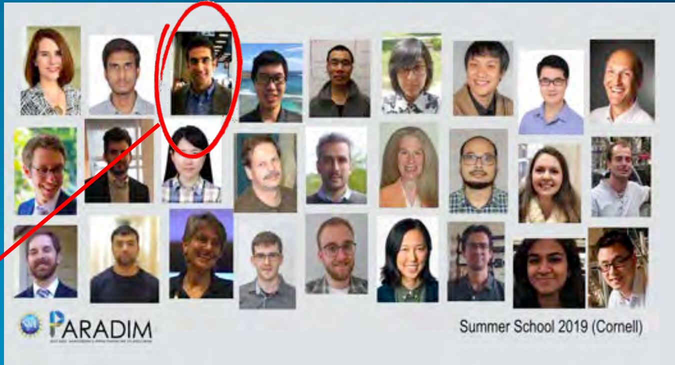
# FAIR Physical Samples

Digital Object Proxy

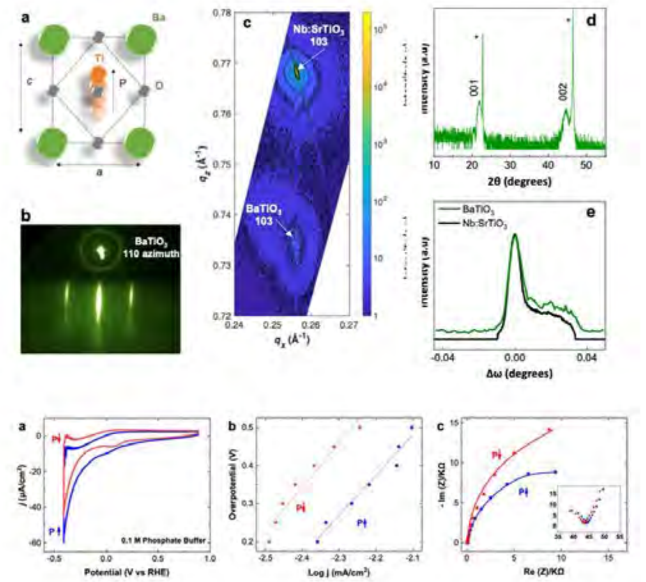
- digital twin
- digital thread
- link to location
- entry point to recreation

Proposal 223 – Dynamic Electrocatalysis on Ferroelectric $BaTiO_3$ Films

- David Fenning, UCSD Nanoengineering Group
- Pedram Abbasi (PhD Student)
- 2019 Summer School "MBE+ARPES: Customizing Oxides…"




Proposal 223: Dynamic Electrocatalysis on Ferroelectric BaTiO3 Films
David Fenning, UCSD




Proposal 223: Abassi et al,. submitted Nature Catalysis

# Training for FAIR
# FAIR for Training

10 Rules for Making Training Materials FAIR

1. Plan
2. Fully Describe
3. Identifier (F)
4. Register
5. Define Access Rules (A)
6. Interoperable Format (I)
7. Reusable for Trainers (license)
8. Reusable for Trainees (metadata) (R)
9. Contribution Friendly
10. Up-to-date


Garcia et al, PLOS Comp Bio, 2020, (https://doi.org/10.1371/journal.pcbi.1007854)

PARADIM
AN NSF MATERIALS INNOVATION PLATFORM
HEMI
HOPKINS EXTREME MATERIALS INSTITUTE

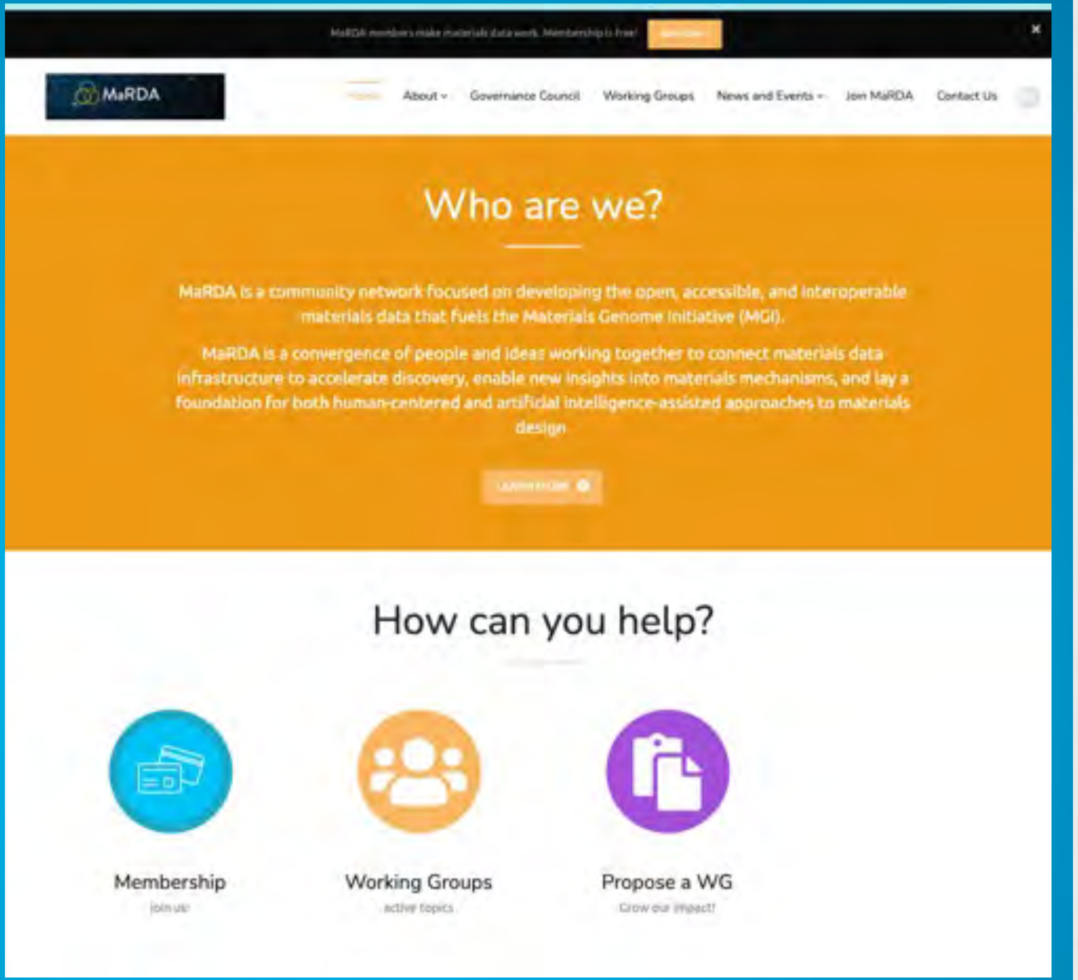
# Community https://marda-alliance.org

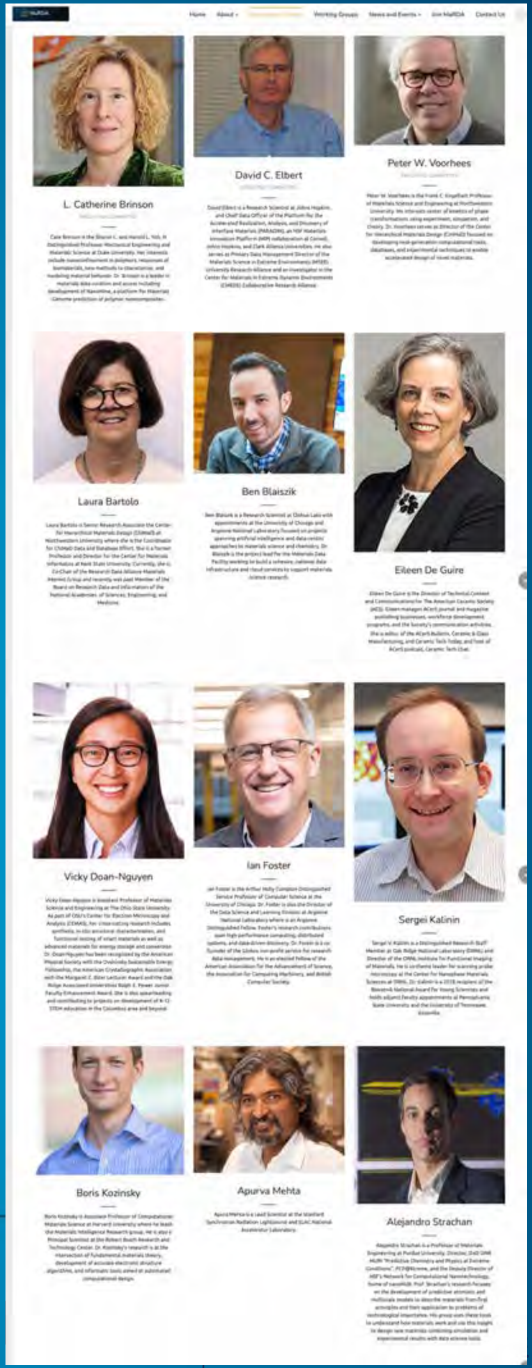
***The Materials Research Data Alliance (MaRDA) is a community-led network focused on connecting and integrating U.S. materials research data infrastructure to realize the promise of open, accessible, and interoperable materials data. Each of these elements are aligned with the goals of the Materials Genome Initiative (MGI). MaRDA provides a platform that promotes the convergence of ideas, people, data, and tools to accelerate discovery, enable new insights into materials mechanisms, and lay the foundation for both human-centered and artificial intelligence-assisted approaches to materials design. MaRDA is governed by an elected council, MaRDAC, that promotes the interests of materials data researchers nationally and internationally, and coordinates the efforts of MaRDA.***

# Community https://marda-alliance.org

## MaRDA: A Year of Building

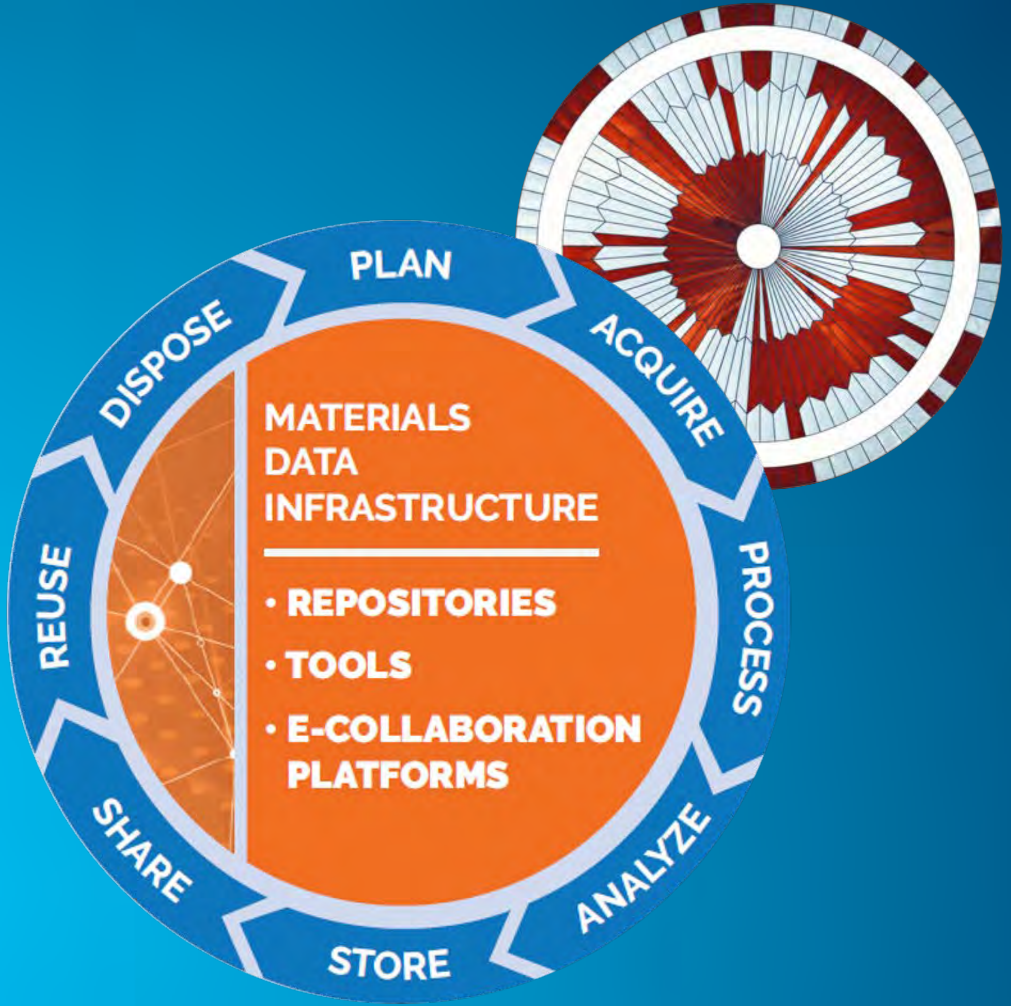
- Founding Council
- Clarification of Mission
- Bylaws
- Website



# Forescasting the FAIR Future

- FAIR is about data use and reuse
  - Data type and purpose are key
  - What do we want to empower?
- Can't be sustained by investigators
  - Expectation yes!  Burden? no!!
  - Scaffold to infrastructure solution
- Materials research is always evolving
  - FAIR cannot be viewed as static
  - Community effort must be sustained
- Reject lock-in
  - Reward connection
  - Incentivize joint success (national/international)
- FAIR is a Community Effort
  - MaRDA  (marda-alliance.org)




TMS 2017 Study
https://doi.org/10.7449/mdistudy_1

How will a PARADIM user 15 years from now leverage the data the platform creates today?

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