# A FAIR Approach to Data and Machine Learning Using *funcX*

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Dane Morgan, Ryan Jacobs, Paul Voyles, Michael Ferris, Jingrui Wei, Xiangguo Li

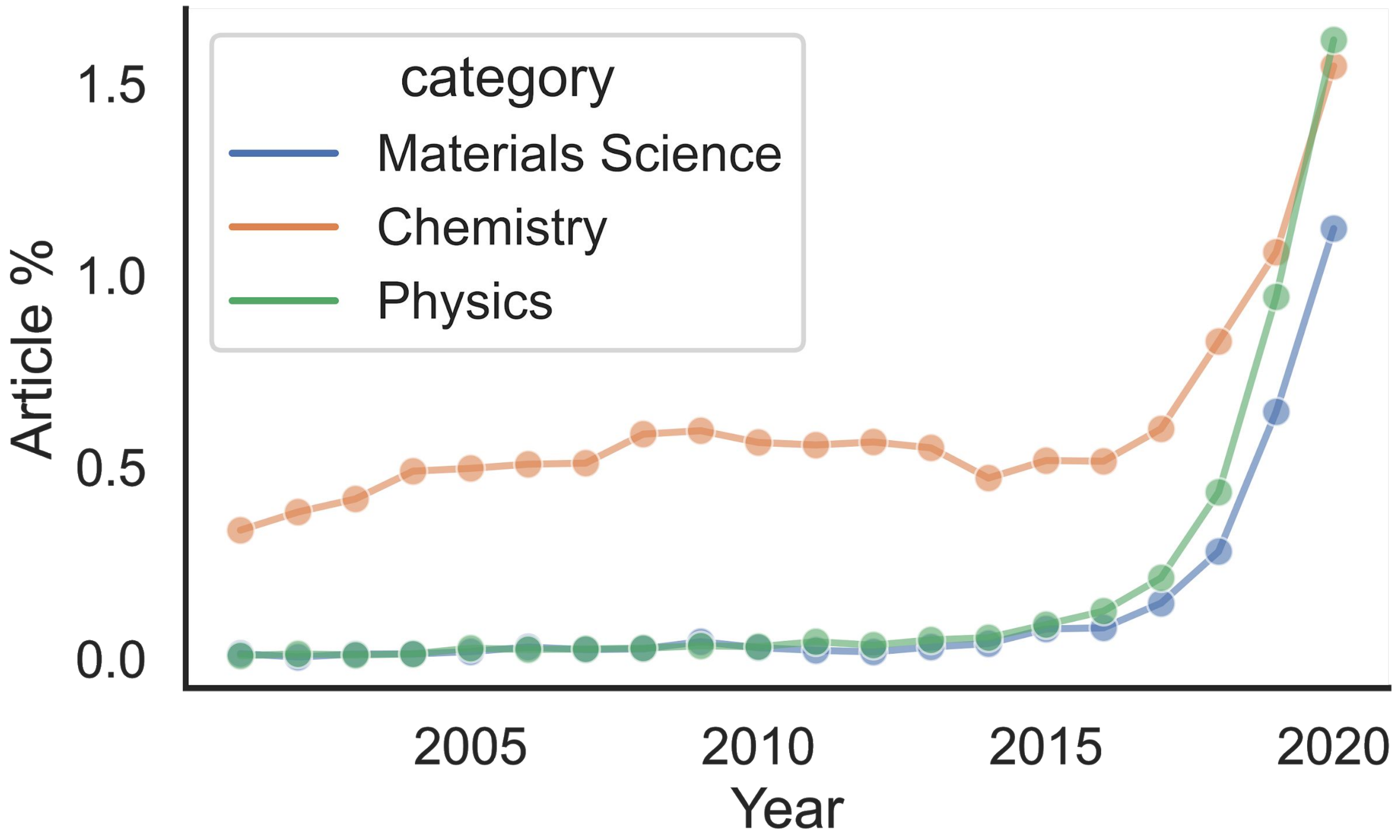
DLHub
Data and Learning Hub for Science
https://www.dlhub.org

**https://www.dlhub.org**

FOUNDRY
DATA, MODELS, SCIENCE

# The Growing Importance of ML and Data in the Sciences

## Data and ML are becoming key drivers of scientific progress




Methods and Data:
https://github.com/blaiszik/ml_publication_charts

# How do we use these models?

## For a given study:

- Where is the code?
- Where are the trained models?
- Where are the training data?
- How can I reproduce these results?

Without all of these pieces, progress is drastically slowed

## Need models and data to be FAIR:

**F**indable
**A**ccessible
**I**nteroperable
**R**eusable

Location of many ML models after a paper is finished

# DLHub for FAIR Models

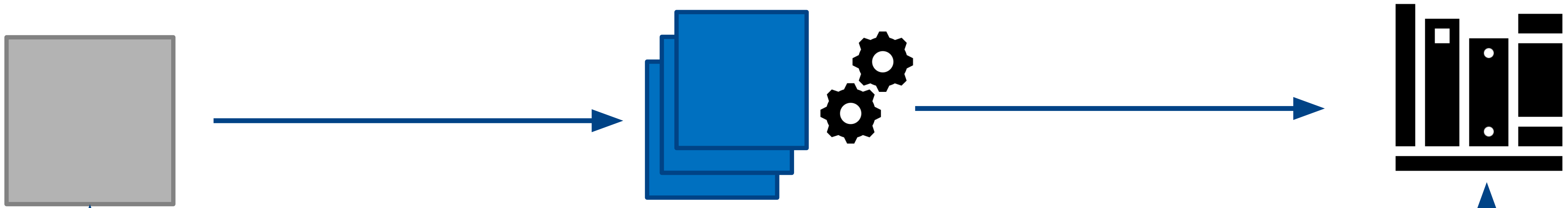
DLHub
Data and Learning Hub for Science
https://www.dlhub.org

## A simple way to find, share, publish, and run machine learning models

### 1 ML Model Submission
- Collect ML models in common formats

### 2 Container Creation
- Create portable containers of models and register in **funcX**

### 3 Model Catalog
- Create a searchable index of data



REST API

### Model Publisher

GitHub, scikit learn, TensorFlow, Keras, PyTorch, python SOFTWARE FOUNDATION

- DOI for citing model
- Landing page
- Run in the cloud
- API to model!

### Model Consumer

python SOFTWARE FOUNDATION, jupyter

REST API

- Find
- Run (in cloud)



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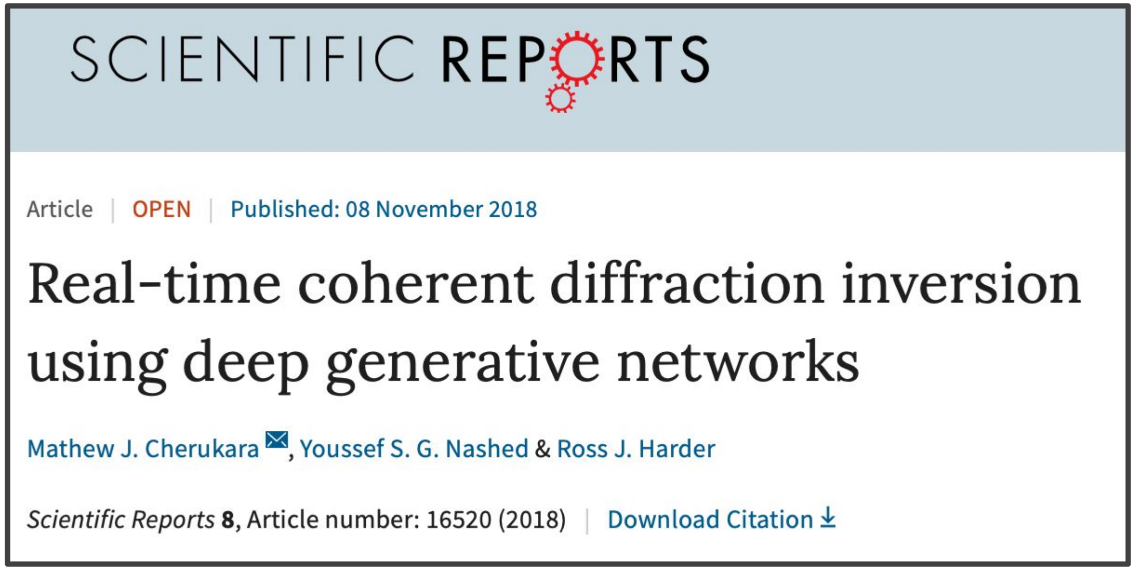
# DLHub Example

- What if I want to evaluate a model from a paper?



SCIENTIFIC REPORTS

Article | OPEN | Published: 08 November 2018

Real-time coherent diffraction inversion using deep generative networks

Mathew J. Cherukara, Youssef S. G. Nashed & Ross J. Harder

*Scientific Reports* **8**, Article number: 16520 (2018) | Download Citation

**DLHub supplies both computational environment and resources**

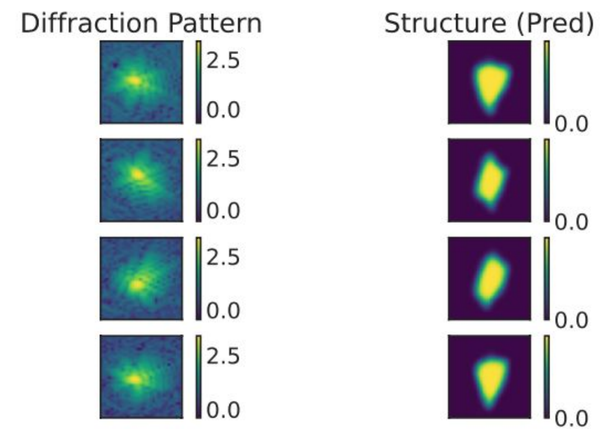
## Run

```
structure_model = "npruyne_globusid/cherukara_structure"
phase_model = "npruyne_globusid/cherukara_phase"

# Load testing data
n_test = 10
intensity_threshold = 0.2
X = ft_test[0:n_test].tolist()

# Call to DLHub to get predictions
intensities = np.asarray(dl.run(structure_model, X))
phases = np.asarray(dl.run(phase_model, X))*2*np.pi-np.pi
```

## Plot and Explore

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# DLHub Containers with funcX

## Container

```
dlhub.json
Dockerfile
maskrcnn_model
model_final.pth
requirements.txt
runtime.txt
```

user-specified

funcx_endpoint
dlhub_sdk
home_run

we then register the container and the function `dlhub_run()` with funcX

dlhub_run(event)

```python
from home_run import create_servable
with open("dlhub.json") as fp:
    shim = create_servable(json.load(fp))
```

dlhub.json contains all servable-specific info

# DLHub Use Case Examples

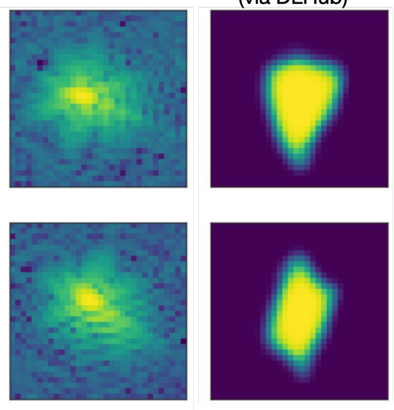
## X-Ray Science

- Predict structure and phase of a material given coherent diffraction intensity
- Data available from Github

```
from dlhub_sdk.client import DLHubClient
dl = DLHubClient()

struct = dl.run("cherukara_structure", X)
```

CDI Intensity | Predicted Structure (via DLHub)

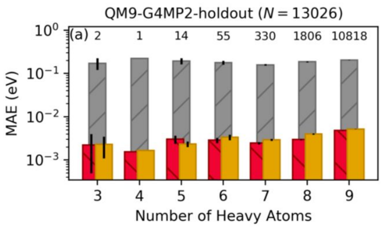


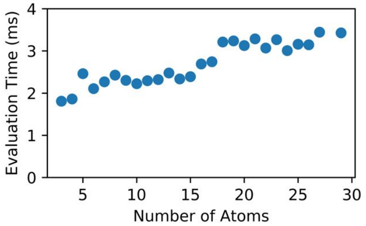
## Energy Storage

- Predict molecular energies with G4MP2 accuracy at B3LYP cost
- Data available in MDF

Machine Learning Prediction of Accurate Atomization Energies of Organic Molecules from Low-Fidelity Quantum Chemical Calculations

Logan Ward[1,2], Ben Blaiszik[1,3], Ian Foster[1,2,3], Rajeev S. Assary[4,5], Badri Narayanan[5,6], Larry Curtiss[4,5]



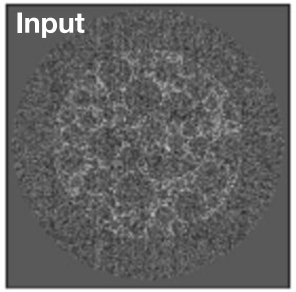



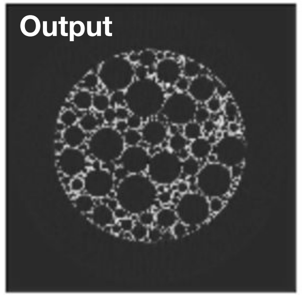

## Tomography

- Enhance tomographic scans and remove noise using generative adversarial model
- Example data available on Petrel

**TomoGAN: Low-Dose X-Ray Tomography with Generative Adversarial Networks**

Zhengchun Liu, Tekin Bicer, Rajkumar Kettimuthu, Doga Gursoy, Francesco De Carlo, Ian Foster



# Foundry Concept

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- Radically reduce the energy barrier to access curated ML datasets and ML models
- Facilitate reuse, meta-studies, benchmarking, and more
- Long term implications for education

Consumers

```
From foundry import Foundry
f = Foundry()

X,y = f.load(“dataset1”, v=“1.0”)
y_pred = f.run(“model1”, v=“1.0”, X)
```

- Models run locally or on distributed endpoints
- Capabilities to pull datasets to desired location or move compute to desired location

Science!

Dataset

Function

API layer

API layer

Data Publishers

Data Provider

Models / Functions

Model Publishers

```
f.data.publish(“./”
“dataset1”, v=“1.1”)
```

```
f.model.publish(“./”
“model1”, v=“1.1”)
```

MATERIALS DATA FACILITY

NIST CHiMaD

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U.S. DEPARTMENT OF ENERGY Argonne NATIONAL LABORATORY

(Dane Morgan, Paul Voyles, Michael Ferris, Marcus Schwarting, Aristana Scourtas, KJ Schmidt, Ben Blaiszik)

NSF WISCONSIN UNIVERSITY OF WISCONSIN–MADISON THE UNIVERSITY OF CHICAGO



NSF CSSI Started Oct. 2019

# Thank You!

DLHub

https://www.dlhub.org

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## Integrative Materials and Design

Northwestern University · Wisconsin · University of Michigan · Illinois · The University of Chicago · Argonne National Laboratory

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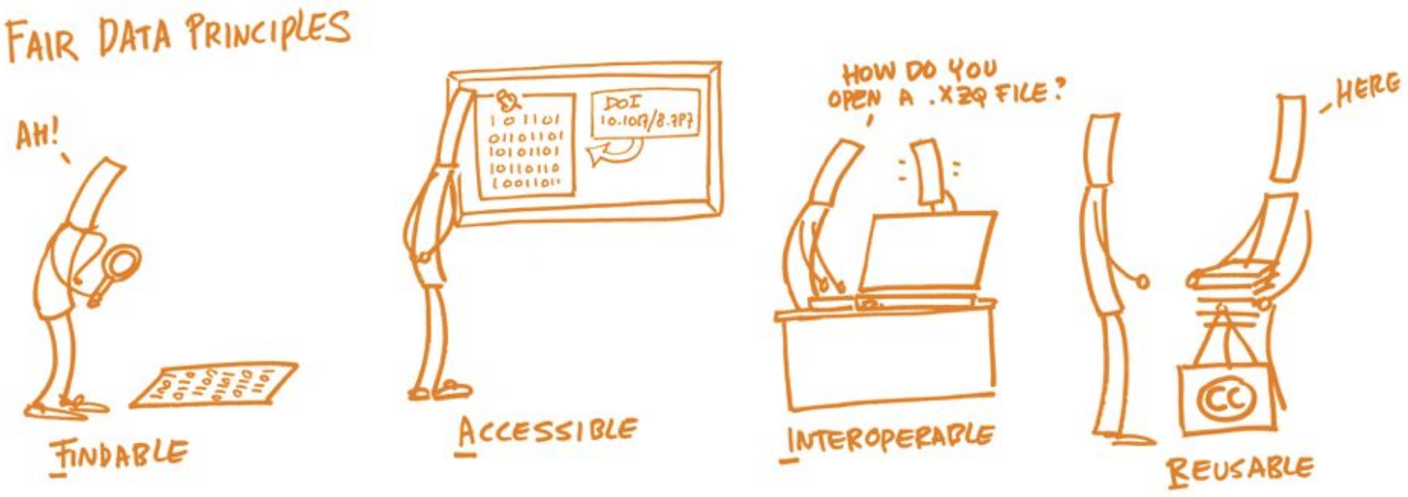
# Backup Slides

# What are FAIR Data Principles?

- Findable
- Accessible
- Interoperable
- Reusable

Set of principles to help make data as useful as possible to the community




https://www.force11.org/group/fairgroup/fairprinciples

What is the state of FAIR data and ML in materials science?

# FAIR Data Principles

## Findable

- Data have an identifier
- Data are registered in a searchable resource

## Accesible

- Data accessible via identifier
- Data retrievable by open protocols

# FAIR Data Principles

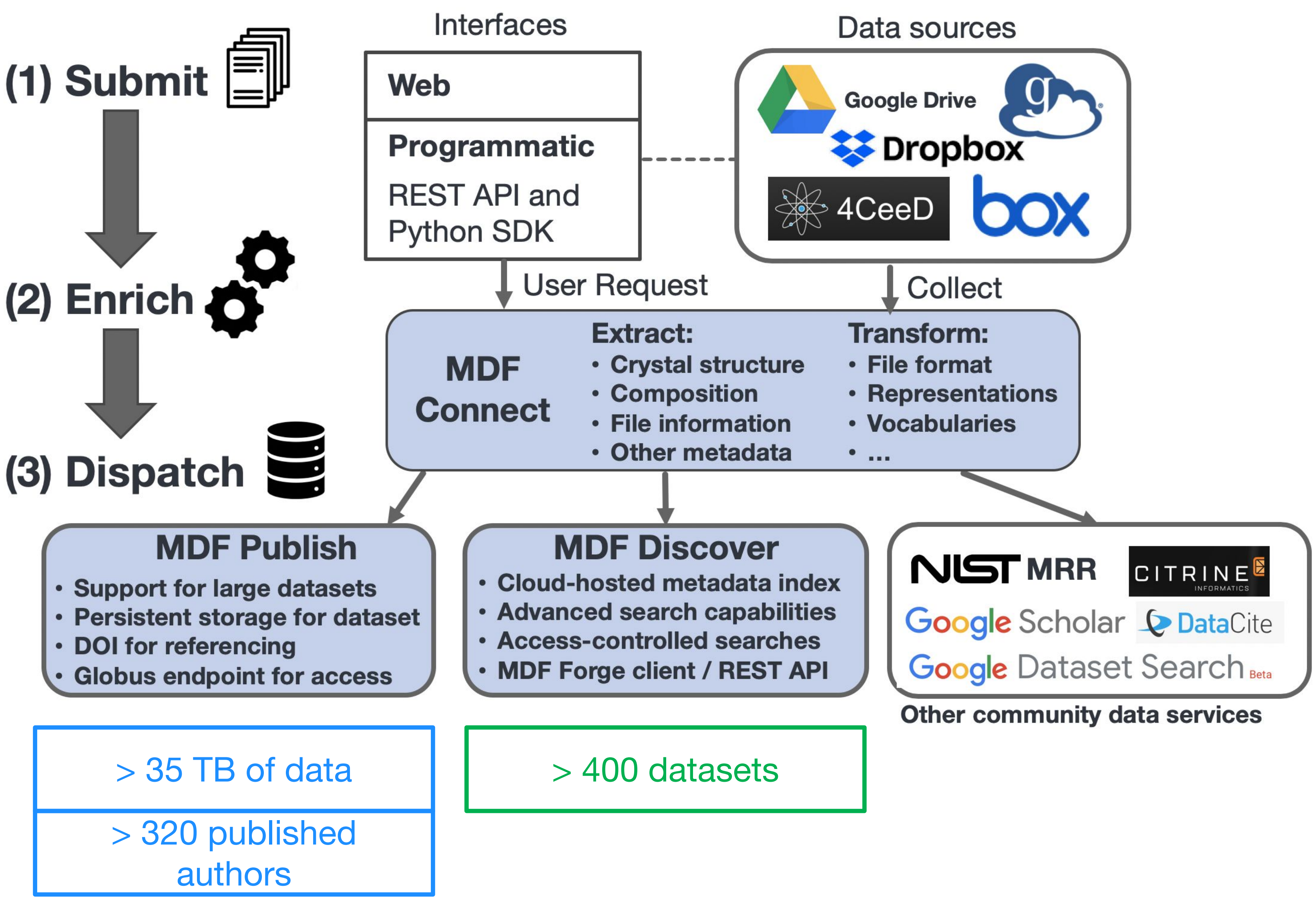
## Interoperable

- Data leverage formalized shared vocabularies
- Vocabularies themselves follow FAIR principles

## Reusable

- Clear licensing
- Descriptive metadata is sufficient to promote reuse

# The Materials Data Facility (MDF)




- Connect: Extract domain-relevant metadata / transform the data
- Publish: Built to handle big data (many TB, millions of files), provides persistent identifier for data, distributed storage enabled
- Discover: Programmatic search index to aggregate and retrieve data across hundreds of indexed data sources

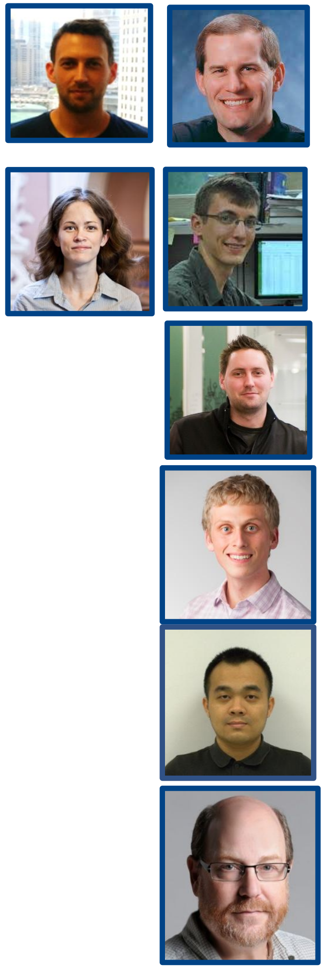
https://www.materialsdatafacility.org

CHiMaD NIST

# The Materials Data Facility

# DATA AND LEARNING HUB FOR SCIENCE (DLHUB)

DLHub



- <u>Collect, publish, categorize</u> models and pre/post processing code
- <u>Operate</u> models as a service to simplify sharing, consumption, and access
- <u>Identify</u> models with unique and persistent identifiers (e.g., DOI)
- <u>Implement</u> versioning, search, access controls etc.

Goal: Deliver FAIR for ML

# DLHub – A Data and Learning Hub for Science

## Describe

- Specify the model files
- Mark up the model with information to make it discoverable and usable

```python
from dlhub_sdk.models.servables.keras import KerasModel
m = KerasModel.create_model("p1b1-example.h5")

m.set_title("CANDLE Pilot 1 - Benchmark 1")
m.set_name("candle_p1b1")
m.set_domains("genomics","biology","HPC")
```

## Publish

- Register with DLHub for containerization as a servable
- DLHub service creates unique endpoint for servable

```python
from dlhub_sdk.client import DLHubClient
dl = DLHubClient()
dl.publish(m)
```

## Discover

- Discover servables with advanced search capabilities through Python SDK or web UI

## Run

- Make predictions by sending data to DLHub and specifying the servable to use

```python
from dlhub_sdk.client import DLHubClient
dl = DLHubClient()
pred = dl.run("candle_p1b1", data)
```

DOI for model

Unique endpoint for each model

Search index for discovery

Python tooling

Ability to run models on distributed compute resources

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# Building on Globus PaaS

- Authentication
- User groups
- Data staging and movement
- Automation capabilities
- Search