



LEADERSHIP  
COMPUTING  
FACILITY

May 27, 2026 | OLCF User Call

# Publishing Research Data with OLCF Constellation

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Data and Platform Services Group, NCCS



U.S. DEPARTMENT  
of **ENERGY**

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FRONTIER



# Data and Platform Services Group



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Information  
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Specialist

Constellation  
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Engineer

Kellen  
Leland

HPC DevOps  
Engineer

Blake  
Nedved

Full Stack  
Software  
Developer

Tatiyanna  
Singleton

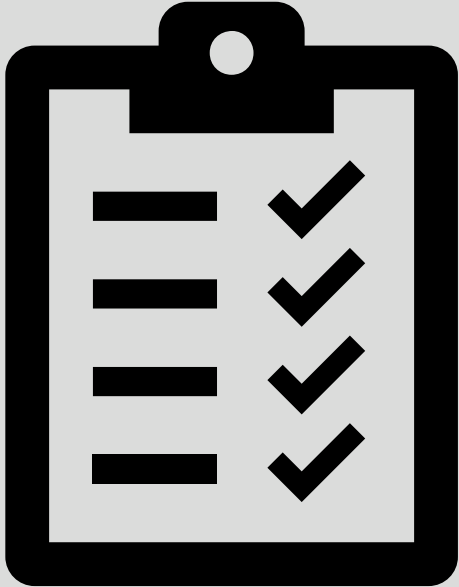
Information  
Science  
Specialist

Constellation  
Curator

Spencer  
Ward

HPC DevOps  
Engineer

# Agenda



- Data Publishing
- Constellation Overview & Workflow
- FAQs
- Site Features & Updates
- Q&A

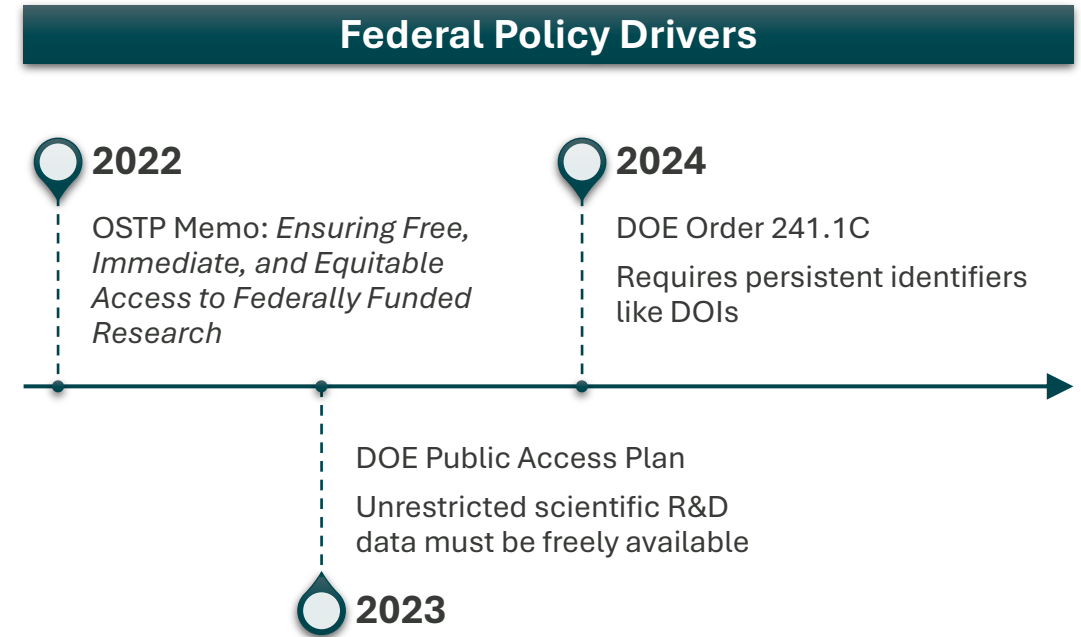
# Data Publishing

## What:

- Publication: making data available for discovery and reuse
- Making data citable and assigning a persistent identifier
- Not the same as sharing or archiving (cold storage)

## Why:

- Funder requirements
- Journal requirements and community norms
- Transparent and reproducible research
- Scientific impact: visibility, reuse, citation



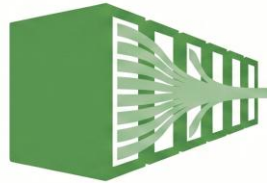
# Constellation Overview



**244 datasets**



**9 million files**



**4.5 PB published data**

largest dataset **2 PB**



© NotebookLM

**A generalist open data repository**  
hosted by OLCF

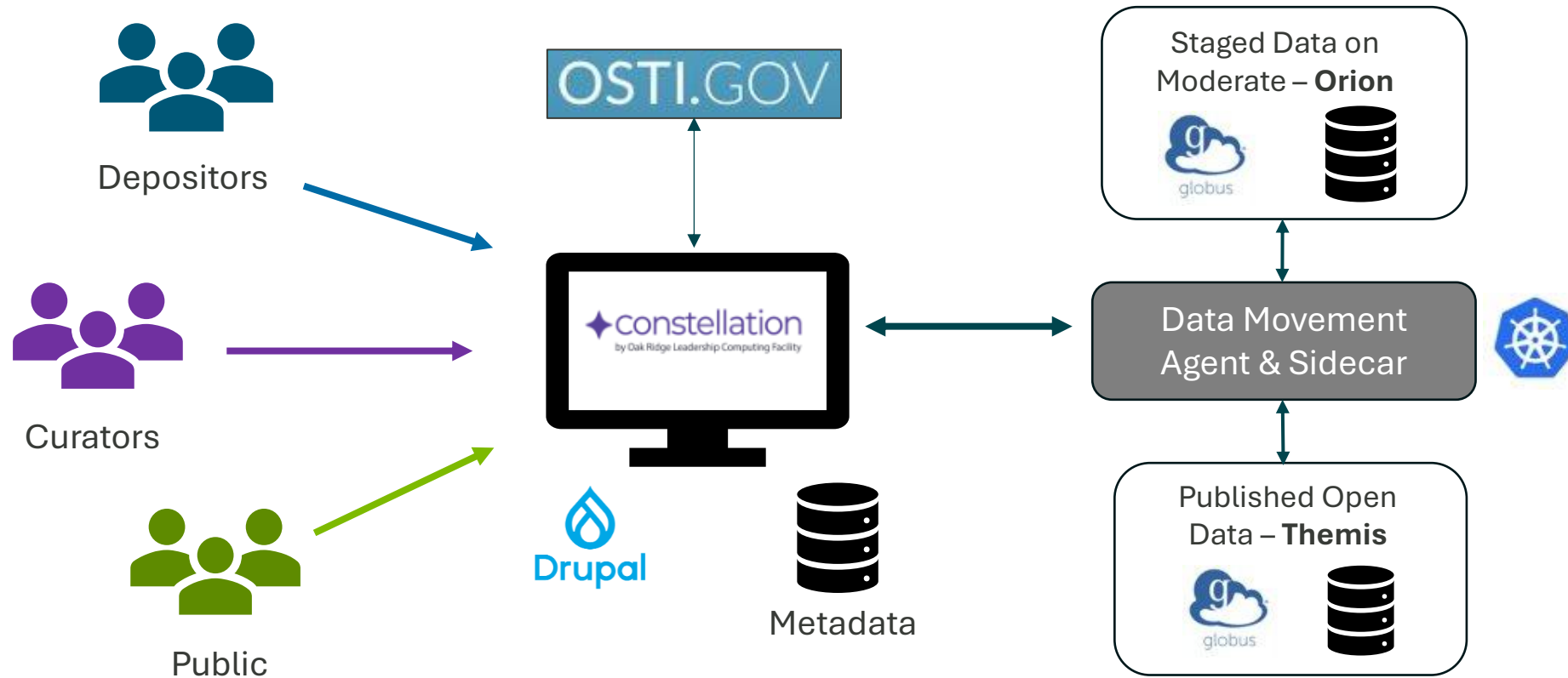
- **Who can deposit:** OLCF facility users + ORNL researchers
- **Who can download:** Anyone (with a Globus account)
- Supports TB-PB scale data
- **DOIs** issued via DOE OSTI Data ID Service

# Constellation Overview

The screenshot shows the homepage of the Constellation dataset repository. At the top left is the Constellation logo, which includes a star icon and the text "constellation by Oak Ridge Leadership Computing Facility". To the right of the logo are navigation links for "Dataset Search", "FAQs", and "Depositor Guide". Further right is a user profile icon. The main content area features a dark purple starry background with white constellation lines. The text "Search the Constellation dataset repository." is centered in white. Below this text are two search input fields: the first is labeled "Title/Author/Description" and the second is labeled "DOI". To the right of these fields is a purple "Search" button. Below the search area is a grey navigation bar with links for "OLCF Help Documentation", "Terms & Conditions", "Accessibility", and "Privacy". At the bottom of the page, the Constellation logo is on the left, and on the right is the Oak Ridge National Laboratory logo with the text "Oak Ridge National Laboratory is managed by UT-Battelle LLC for the US Department of Energy".

<https://doi.ccs.ornl.gov/>

# Constellation Overview



# What Constellation is and isn't



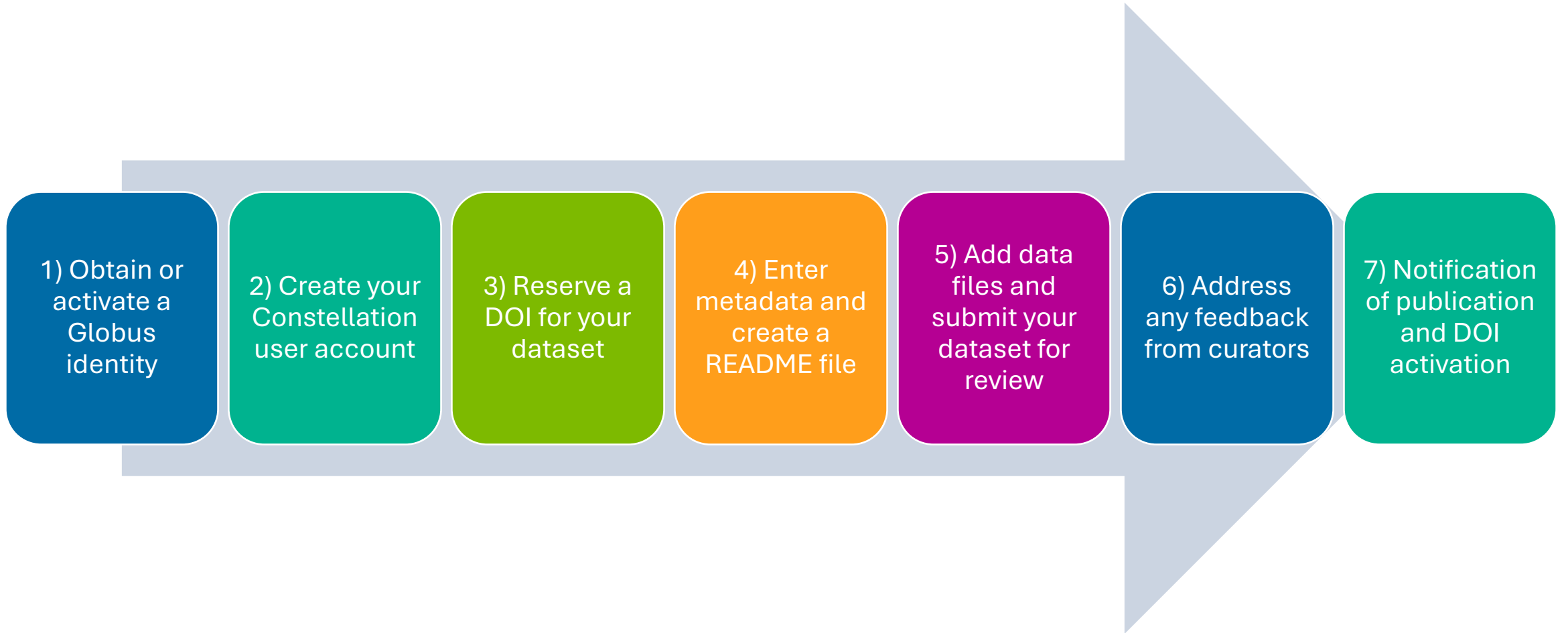
- A data repository for making research results public
- A data repository for hosting **big** open-access datasets
- A generalist repository with built-in support for metadata that meets OSTI requirements



- Additional archival storage for project data
- A data sharing platform for collaborative work
- A domain-specific repository for hosting datasets in particular formats (e.g., gene expression data)
- A secure repository for hosting PII/PHI/CUI data

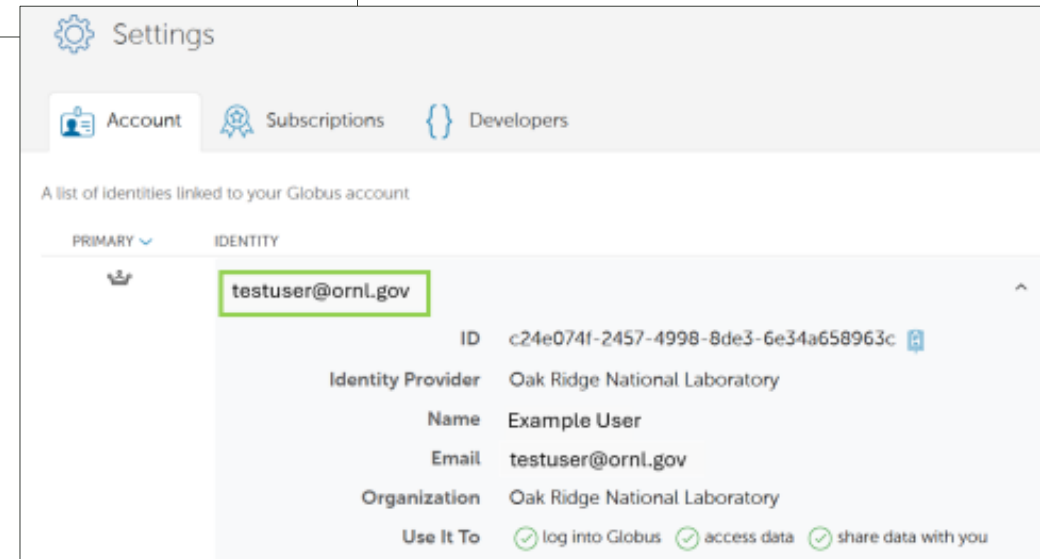
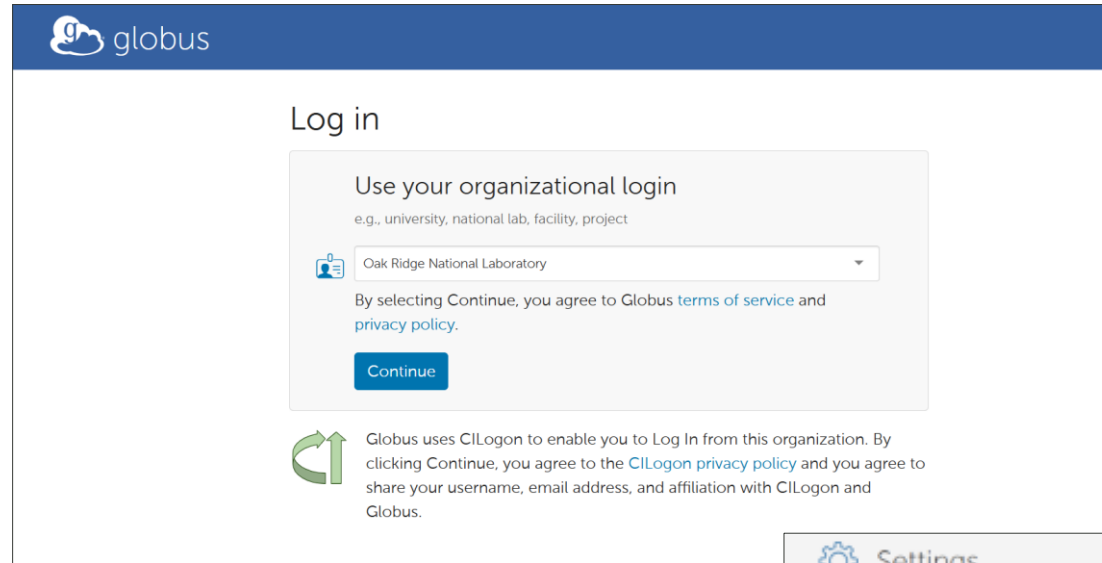
# How to publish data

# Publication Process



# Publication Process

1) Obtain or activate a Globus identity



# Publication Process

2) Create your Constellation user account

constellation by Oak Ridge Leadership Computing Facility

Dataset Search FAQs Depositor Guide Login

**Constellation Upgrade Notification**

Constellation will be experiencing upgrades at 11:30am - 12:30pm Eastern on May 26th, 2026 and may be inaccessible during this time.

We apologize for any inconvenience. Please reach out to [doi\\_support@ornl.gov](mailto:doi_support@ornl.gov) with any questions.

Search the Constellation dataset repository.

Title/Author/Description DOI Search

OLCF Help Documentation Terms & Conditions Accessibility Privacy

constellation by Oak Ridge Leadership Computing Facility

Oak Ridge National Laboratory is managed by UT-Battelle LLC for the US Department of Energy

## Sign in to your account

You can access your account by signing in with one of the options below.

Log in with OLCF

Log in with UCAMS/XCAMS

### Need help?

For help signing in with Single Sign On, please contact OLCF support.

Contact OLCF support

## On first login:

- Enter Globus identity
- Accept depositor agreement

# Publication Process

3) Reserve a DOI for your dataset

+ Create New DOI Reservation

### Reserve DOI

Reserving a DOI creates a draft record. Add a title now, then continue editing metadata on the editor page.

Title \*

Enter the provisional title of your dataset for use in the DOI reservation. You may change the title before publication.

Was any part of this dataset created on resources at the Oak Ridge Leadership Computing Facility (OLCF)? \*

OLCF resources include Frontier, Summit, Titan, Slate (Onyx, Marble), Andes, etc.

No

Yes

Save

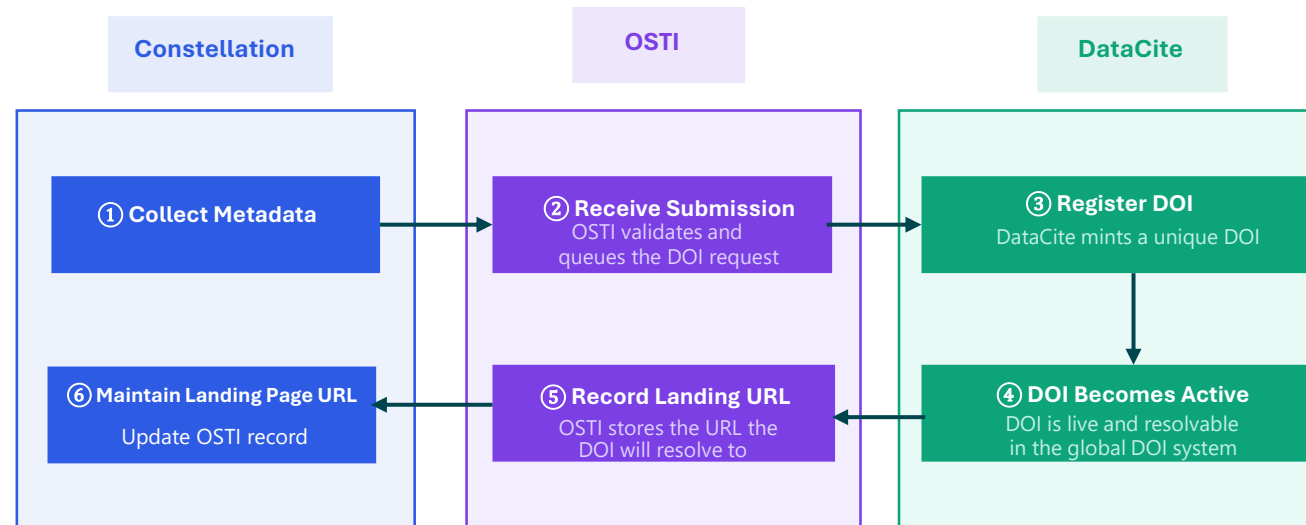
- **Congratulations**  
Your reservation was successful!  
"Data for "Signatures of Thermoreversible Associations in X-ray and Neutron Scattering from Dilute Polyzwitterion Solutions"" has been reserved with OSTI and is:  
**10.13139/ORNLNCCS/3187500**
- **What's next?**  
Before you can submit your DOI for publishing, you need to add required metadata and upload your datasets.
- New DOI Status [Data for "Signatures of Thermoreversible Associations in X-ray and Neutron Scattering from Dilute Polyzwitterion Solutions"](#) has been created.

Reserved DOIs are placeholders within the OSTI e-link ingest system but are not yet registered at DataCite. Reserved DOIs won't resolve at <https://dx.doi.org> and won't be publicly available in [osti.gov](https://www.osti.gov), DOE Data Explorer, or major commercial search engines such as Google.

# Using a DOI

Digital Object Identifiers make scholarly outputs citable:

- A persistent pointer *to a landing page*
- Enables linking, tracking, and discoverability
- Should be used instead of a URL in data availability statements
- Constellation mints DOIs via DOE OSTI



# Publication Process

4) Add metadata and create a README file

[Test Dataset 2](#) Draft Edit  
10.13139/ORNLNCCS/3187403 • May 13, 2026

Minimum Required Fields	Recommended Fields
Author Names and Affiliations	Author ORCID IDs
DOE Sponsoring Organizations	Contributing Organizations
Originating Research Organization	Other Funding/Contract Numbers
DOE Contract Number	Topic (Subject)
OLCF Project Identifier	Keyword Tags
Dataset Type	Software Needed
Description	Related Identifiers

# Publication Process

4) Add metadata and create a README file

```
This readme file was generated on [YYYY-MM-DD] by [NAME]

GENERAL INFORMATION

1. Title of Dataset:

2. Author Information
  A. Principal Investigator Contact Information
     Name:
     ORCID:
     Institution:
     Email:

  B. Associate or Co-investigator Contact Information
     Name:
     ORCID:
     Institution:
     Email:

  C. Alternate Contact Information
     Name:
     ORCID:
     Institution:
     Email:

3. Date of data collection: <provide single date, range, or approximate date; suggested format YYYY-MM-DD>

4. Geographic location of data collection: <provide latitude, longitude, or city/region, State, Country, as

5. Information about funding sources that supported the collection of the data:

SHARING/ACCESS INFORMATION

1. Reuse restrictions placed on the data:

2. Links to publications that cite or use the data:

3. Links to other publicly accessible locations of the data:

4. Links/relationships to ancillary data sets:

5. Was data derived from another source? If yes, list source(s):

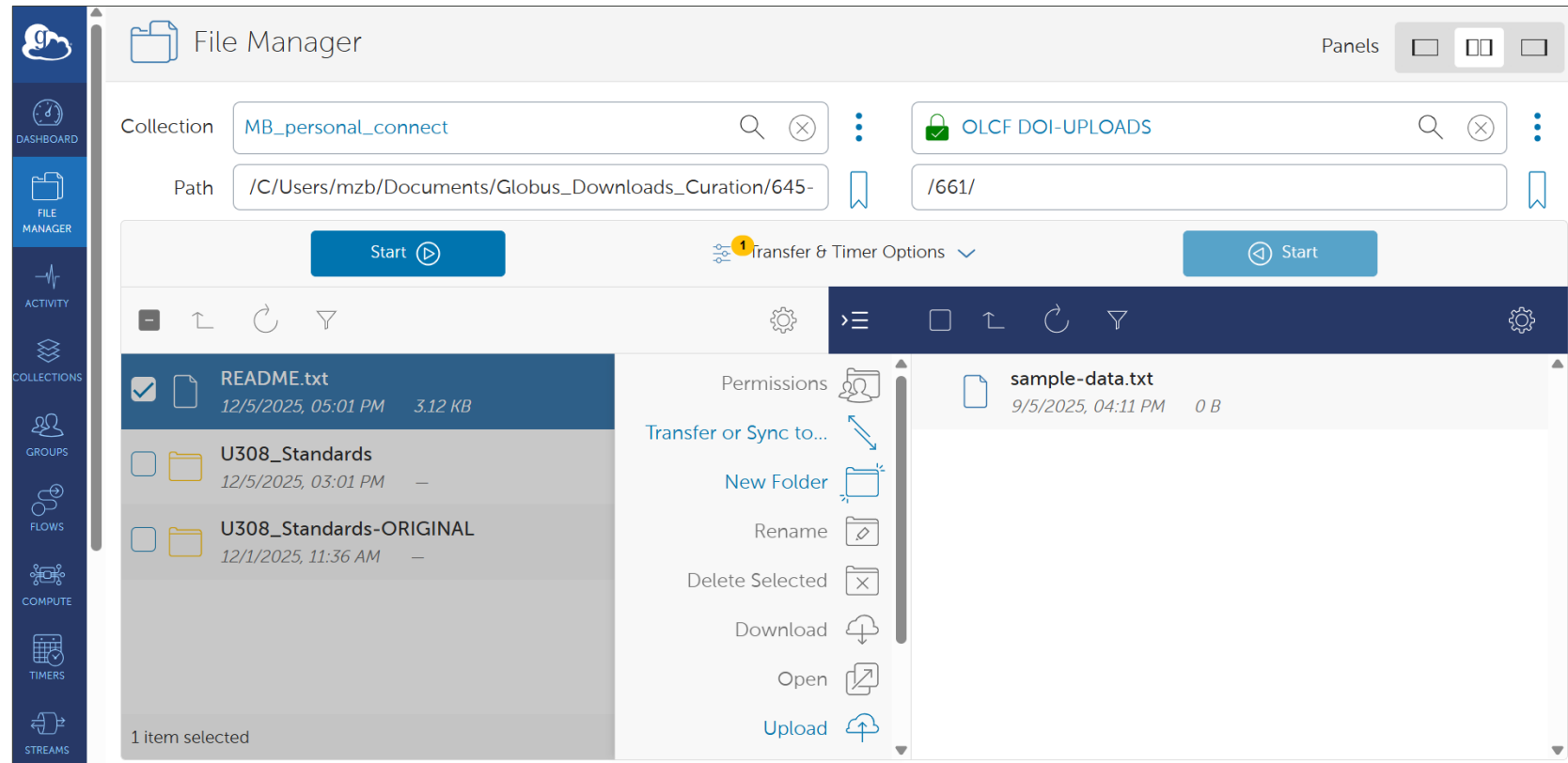
6. Recommended citation for this dataset:
```

- README templates available on Constellation
- Important reuse information
- Data & file overview
- Methodological information
- Variable list

# Publication Process

5) Add data files and submit your dataset for review

Upload with Globus 

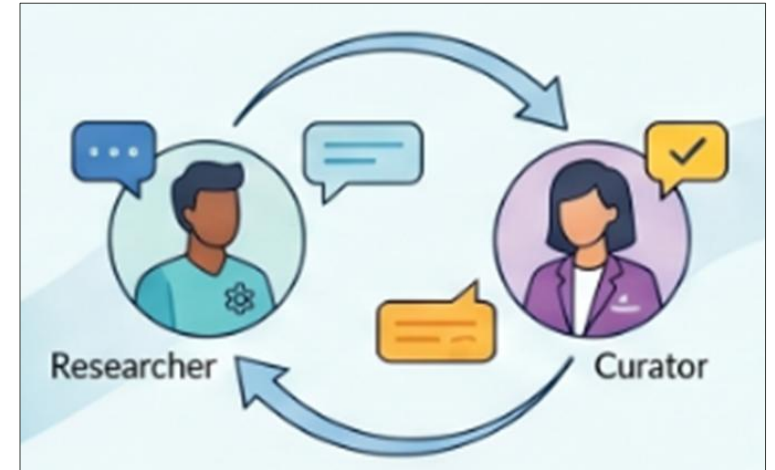


The screenshot displays the Globus File Manager interface. The main window shows a collection named 'MB\_personal\_connect' with a path of '/C/Users/mzb/Documents/Globus\_Downloads\_Curation/645-'. A secondary path '/661/' is also visible. The interface includes a 'Start' button and a 'Transfer & Timer Options' dropdown menu. The file list shows a selected file 'README.txt' (3.12 KB) and two folders: 'U308\_Standards' and 'U308\_Standards-ORIGINAL'. A context menu is open over the selected file, listing actions such as 'Permissions', 'Transfer or Sync to...', 'New Folder', 'Rename', 'Delete Selected', 'Download', 'Open', and 'Upload'. The 'Upload' option is highlighted. The interface also features a sidebar with navigation options like 'Dashboard', 'File Manager', 'Activity', 'Collections', 'Groups', 'Flows', 'Compute', 'Timers', and 'Streams'.

# Publication Process

6) Address any questions or concerns from curators

- Submissions are reviewed for completeness and quality of documentation
  - README
  - File manifest
  - Code checks
- FAIR: Findable, Accessible, Interoperable, Reusable
- Checks for sensitive data
- Reviewing and enriching metadata



# Preparing data for publication

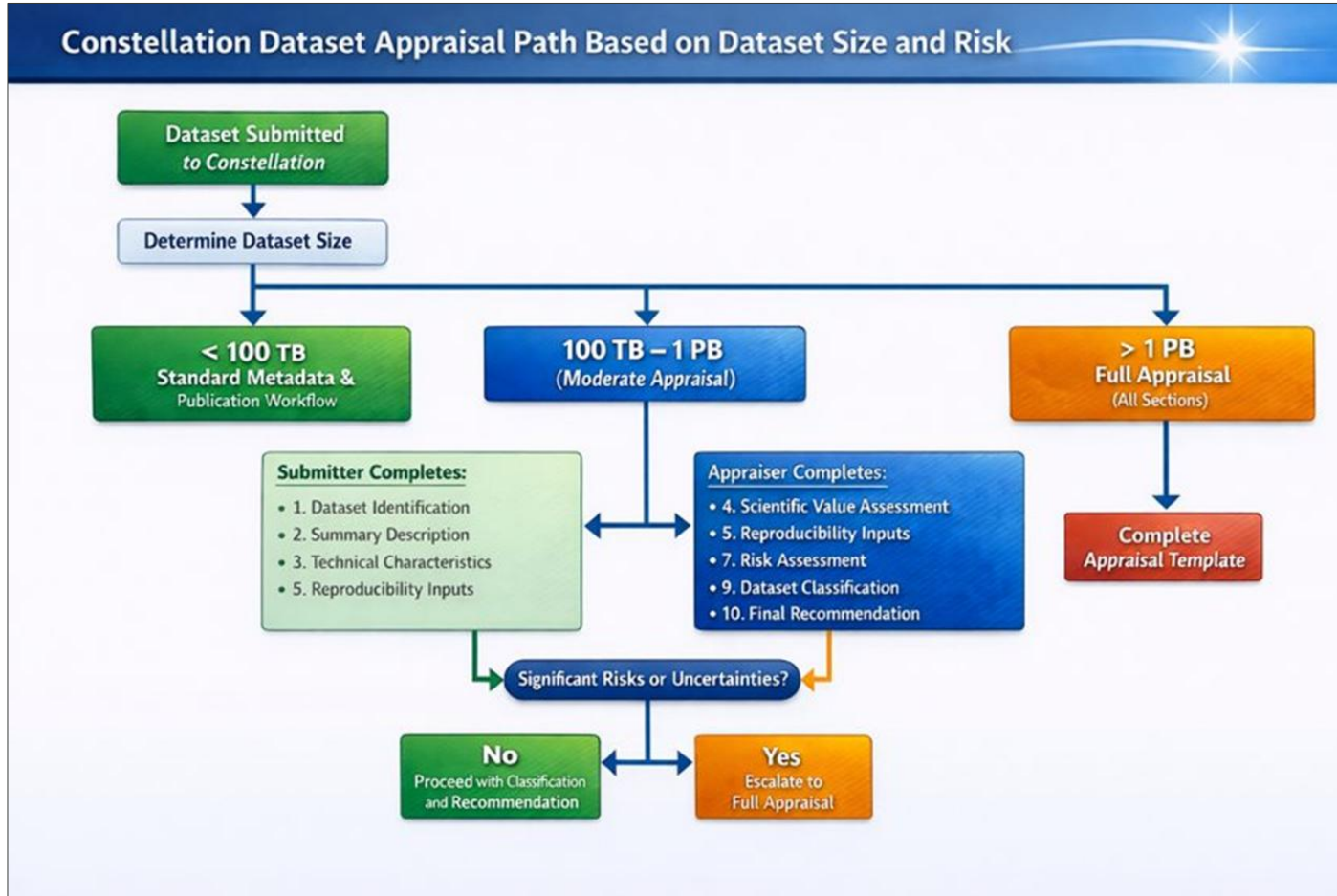
## File formats

- Prefer open, documented formats (HDF, NetCDF, CSV, PNG, etc.)
- Proprietary formats: confirm redistribution rights, provide usage notes
- Consider AI readiness: consistent structures and schemas

## Sensitive OLCF Data

- Remove/anonymize project identifiers, usernames, file paths
- Check included log files
- Check absolute paths included in code

# Large Dataset Appraisal



- Applies to datasets >100 TB
- Collaborative appraisal between depositor, RUC, domain experts, and curator

# Publication Process

7)  
Notification  
of publication  
and DOI  
activation

OSTI.GOV / Search for HfZr\_BCC\_SolidSolution\_128atoms\_VASP6 / Dataset: HfZr\_BCC\_SolidSolution\_128atoms\_VASP6

## HfZr\_BCC\_SolidSolution\_128atoms\_VASP6

DATASET · 16 October 2025

DOI: <https://doi.org/10.13139/OLCF/2998298> · OSTI ID: 2998298

Lupo Pasini, Massimiliano <sup>[1]</sup>; Choi, Jong Youl <sup>[1]</sup>

+ Show Author Affiliations

We performed density functional theory (DFT) calculations for body-centered-cubic (BCC) structures with 128 lattices sites of solid solution binary alloys hafnium-zirconium (Hf-Zr). The electronic structures of alloys have been calculated using Vienna Ab initio Simulation Package (VASP). Within this package the DFT approach is used to reduce many-body Schrodinger equation to set of single particle Kohn-Sham (KS) equations. The generalized electronic exchange-correlation functional is described by Perdew-Burke-Ernzerhof parametrization. The electron-ion interactions is described by pseudopotentials developed within the plane-wave basis projector augmented-wave (PAW) approach. These pseudopotentials are available at the VASP portal (<http://cms.mpi.univie.ac.at/vasp/>). Our calculations have been run with the pseudopotentials treating s and p semi-core states as valence in case for the elements Hf and Zr. The electronic densities and potentials are expanded over plane-waves with energy cutoff of 350 eV. 2x2x2 k-mesh and normal precision were used. The alloys were modeled by supercell containing 128 randomly distributed atoms. At initial step the atoms occupy perfect bcc lattice sites. This initial structure was optimized until energy changes less than 1e-6 eV, while forces acting on atoms don't exceed 1e-2 eV/angstrom. The electron-ion interaction is described by PAW pseudopotentials. The calculations have been collected by sampling chemical compositions across the entire compositional range. The chemical compositions have been sampled by progressively changing the number of atoms per constituent by 4. For each chemical composition of binaries and ternaries, the first-principle calculations have been run for 100 randomized arrangements of the constituents on the BCC lattice sites. We collected data for a total of 3,100 randomized atomic structures over 31 chemical compositions.

[View Dataset](#) [Cite](#) [Export](#) [Share](#) [Save](#)

Details		Similar Records / Subjects	
Research Organization:	Oak Ridge National Laboratory (ORNL), Oak Ridge, TN (United States)		
Sponsoring Organization:	Office of Science (SC)		
DOE Contract Number:	AC05-00OR22725		
OSTI ID:	2998298		

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by Oak Ridge Leadership Computing Facility

Dataset Search FAQs Depositor Guide [Login](#)

[Home](#) > [Dataset](#)

## HfZr\_BCC\_SolidSolution\_128atoms\_VASP6

Massimiliano Lupo Pasini | Oak Ridge National Laboratory  
Jong Youl Choi | Oak Ridge National Laboratory

[Download Dataset on Globus](#)

### Description

We performed density functional theory (DFT) calculations for body-centered-cubic (BCC) structures with 128 lattices sites of solid solution binary alloys hafnium-zirconium (Hf-Zr). The electronic structures of alloys have been calculated using Vienna Ab initio Simulation Package (VASP). Within this package the DFT approach is used to reduce many-body Schrodinger equation to set of single particle Kohn-Sham (KS) equations. The generalized electronic exchange-correlation functional is described by Perdew-Burke-Ernzerhof parametrization. The electron-ion interactions is described by pseudopotentials developed within the plane-wave basis projector augmented-wave (PAW) approach. These pseudopotentials are available at the VASP portal (<http://cms.mpi.univie.ac.at/vasp/>). Our calculations have been run with the pseudopotentials treating s and p semi-core states as valence in case for the elements Hf and Zr. The electronic densities and potentials are expanded over plane-waves with energy cutoff of 350 eV. 2x2x2 k-mesh and normal precision were used. The alloys were modeled by supercell containing 128 randomly distributed atoms. At initial step the atoms occupy perfect bcc lattice sites. This initial structure was optimized until energy changes less than 1e-6 eV, while forces acting on atoms don't exceed 1e-2 eV/angstrom. The electron-ion interaction is described by PAW pseudopotentials. The calculations have been collected by sampling chemical compositions across the entire compositional range. The chemical compositions have been sampled by progressively changing the number of atoms per constituent by 4. For each chemical composition of binaries and ternaries, the first-principle calculations have been run for 100 randomized arrangements of the constituents on the BCC lattice sites. We collected data for a total of 3,100 randomized atomic structures over 31 chemical compositions.

### Details

DOI: <https://doi.org/10.13139/OLCF/2998298>

Release Date  
October 16, 2025

Subject  
74 ATOMIC AND MOLECULAR PHYSICS, 71 CLASSICAL AND QUANTUM MECHANICS, GENERAL PHYSICS, 75 CONDENSED MATTER PHYSICS, SUPERCONDUCTIVITY AND SUPERFLUIDITY, 37 INORGANIC, ORGANIC, PHYSICAL, AND ANALYTICAL CHEMISTRY, 36 MATERIALS SCIENCE

Keywords  
Machine Learning, Solid Solution Alloys, Density Functional Theory, First Principles

### Dataset

Dataset Type  
ND Numeric Data

Software  
Python

# How to get help

## OLCF User Documentation

Need Help? Contact us.  
help@olcf.ornl.gov

Search docs

- Contact & Support
- Accounts and Projects
- Connecting
- Systems
- Services and Applications
  - Slate
  - myOLCF
  - Jupyter
  - Data Publication (Constellation)
    - Constellation Overview
    - Infrastructure
    - Authentication and Account Setup
    - Preparing and Submitting Data
    - Reusing Constellation Data
  - S3M
  - OLCF Inference Service Documentation
- Data Storage and Transfers
- Software
- Training
- Quantum
- Scalable Protected Infrastructure (SPI)
- Advanced Computing Ecosystem Testbed (ACE)

Home / Services and Applications / Data Publication (Constellation)  
[Edit on GitHub](#) | [OLCF Home Page](#) | [myOLCF](#)

## Data Publication (Constellation)

- Constellation Overview
- Infrastructure
- Authentication and Account Setup
- Preparing and Submitting Data
  - Preparing Your Dataset
  - Data Review and Release
  - Reserving a Draft DOI
  - Removal of Dataset Drafts
  - Adding Data and Documentation
  - Review States
  - Data Curation
- Reusing Constellation Data

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Built with [Sphinx](#) using a [theme](#) provided by [Read the Docs](#).

[https://docs.olcf.ornl.gov/services\\_and\\_applications/constellation/index.html](https://docs.olcf.ornl.gov/services_and_applications/constellation/index.html)

## Constellation Depositor Guide

constellation  
by Oak Ridge Leadership Computing Facility

Dataset Search FAQs **Depositor Guide** Login

[Home](#)

## Data Depositor Guide

Welcome! Constellation is a research data repository service of the Oak Ridge Leadership Computing Facility (OLCF), available for OLCF users as well as Oak Ridge National Laboratory (ORNL) staff. Datasets published in Constellation are assigned a Digital Object Identifier (DOI) by the DOE Office of Scientific and Technical Information (OSTI) and reported for inclusion in the [DOE Data Explorer](#). Constellation can assist projects in meeting the objectives of the 2023 DOE Public Access Plan for federally funded research.

Data submitted to this repository may be the results of research:

- 1) conducted using a project allocation on OLCF resources including Frontier, Summit, Slate, Andes, etc., or
- 2) funded wholly or in part by the US Department of Energy under its contract with UT-Battelle, LLC (DE-AC05-00OR22725) for the management of ORNL.

For questions and help with data deposits, email [doi\\_support@ornl.gov](mailto:doi_support@ornl.gov).

### Steps to publish a dataset in Constellation

There are seven steps involved in submitting and publishing your dataset on Constellation:

1. Obtain or activate a Globus identity
2. Create your Constellation user account
3. Reserve a DOI for your dataset
4. Add metadata and create a README file
5. Add data files and submit your dataset for review
6. Address any questions or concerns about your dataset received from ORNL curators
7. Receive notification that your dataset has been published

See "Detailed submission instructions" below for more information on each step.

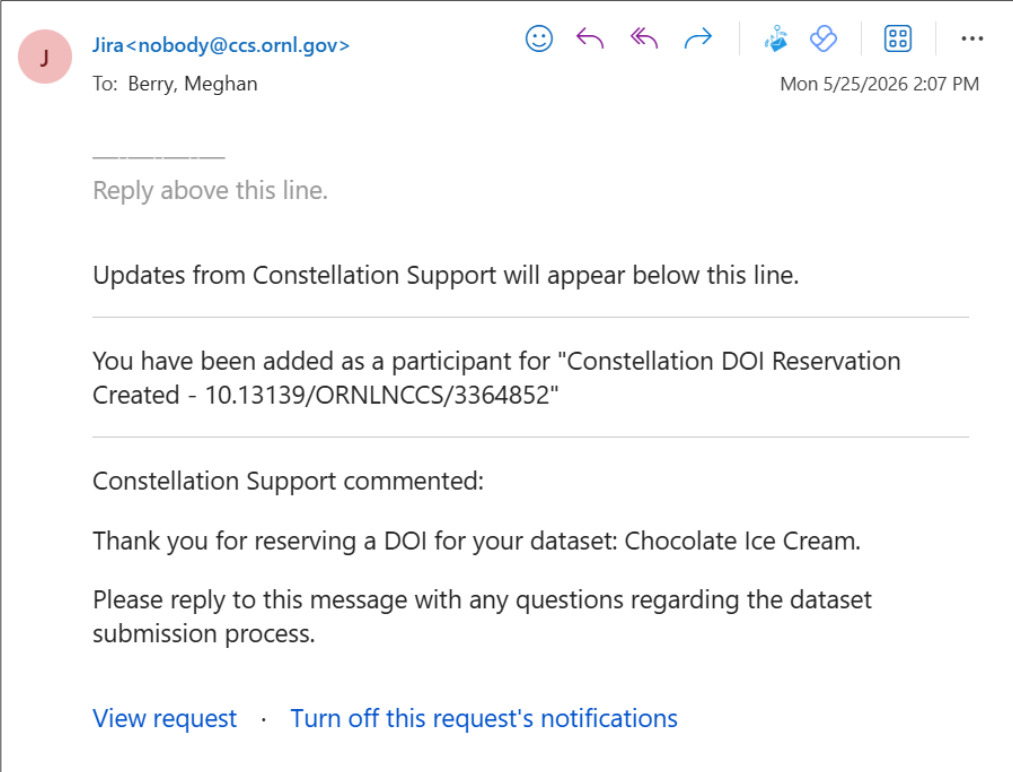
Data depositors are responsible for understanding the licensing and reuse terms of any input datasets.

**NOTE:** Staff members of Oak Ridge National Laboratory should also follow relevant SBMS procedures to [Review and Release Scientific and Technical Information](#). A submission workflow for datasets is available in RESolution, where submitters will be asked to provide the DOI that has been reserved in Constellation. Datasets should be

<https://doi.ccs.ornl.gov/data-depositor-guide>

# How to get help

- Email confirmation of DOI reservation
- Reply to reach a curator directly
- Submit a ticket to OLCF User Assistance ([help@olcf.ornl.gov](mailto:help@olcf.ornl.gov))



Jira <nobody@ccs.ornl.gov>  
To: Berry, Meghan  
Mon 5/25/2026 2:07 PM

-----  
Reply above this line.

Updates from Constellation Support will appear below this line.

You have been added as a participant for "Constellation DOI Reservation Created - 10.13139/ORNLNCCS/3364852"

Constellation Support commented:

Thank you for reserving a DOI for your dataset: Chocolate Ice Cream.

Please reply to this message with any questions regarding the dataset submission process.

[View request](#) · [Turn off this request's notifications](#)

# FAQs

## ***What licenses can I apply to my dataset?***

- Depends on ORNL staff status
- Generally, no license – data is ‘free to use and reuse’
- Staff can work with you to meet journal requirements
- Authors are responsible for understanding third-party licenses

## ***Does Constellation support blind review of data?***

- No, data is not viewable until fully public with author names
- Data can be hosted elsewhere (Zenodo, Anonymous GitHub) temporarily

## ***How do I update or version an existing publication?***



- Minor updates and additions can be made to the same DOI
- Major revisions and corrections should have a new DOI
- The version number should be part of the title
- Metadata can be updated anytime

## ***Is Constellation a substitute for the standard review and release process?***

- No, authors are responsible for following institutional release standards (RESolution)

# Site Features & Updates

# User dashboard

by Oak Ridge Leadership Computing Facility[Dataset Search](#) [FAQs](#) [Depositor Guide](#) 

[Home](#) [+ Create New DOI Reservation](#)

## Welcome back, Mzb!

From your dashboard you have access to create new DOI reservations, edit your datasets, and view your published datasets.

### Latest Activity

<a href="#">Test Dataset 2</a> 10.13139/ORNLNCCS/3187403 • May 13, 2026	<a href="#">Draft</a>	<a href="#">Edit</a>
<a href="#">Test Donut Dataset</a> 10.13139/OLCF/3187457 • May 15, 2026	<a href="#">Draft</a>	<a href="#">Edit</a>
<a href="#">Gumdrop Sequence Data</a> 10.13139/OLCF/2568425 • June 3, 2025	<a href="#">Draft</a>	<a href="#">Edit</a>
<a href="#">Melted Asphalt</a> 10.13139/ORNLNCCS/1974168 • August 22, 2025	<a href="#">Draft</a>	<a href="#">Edit</a>

# My Datasets page

constellation  
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Dataset Search   FAQs   Depositor Guide

Home   [+ Create New DOI Reservation](#)

## My Datasets

Datasets 6 datasets   Search   Filter

Title	DOI	Started on	Submitted on	Status
<a href="#">Test Donut Dataset</a>	10.13139/OLCF/3187457	5/15/26 9:31 AM	—	Draft
<a href="#">Test Dataset 2</a>	10.13139/ORNLNCCS/3187403	5/13/26 12:13 PM	5/13/26 12:32 PM	Draft
<a href="#">The ECMWF IFS Experimental Nature Run at 1-km (XNR1K)</a>	10.13139/OLCF/2308754	8/8/25 10:46 AM	—	Draft
<a href="#">Melted Asphalt</a>	10.13139/ORNLNCCS/1974168	8/8/25 10:09 AM	—	Draft

Submitted on

Search   Filter

**Filters** ✕

Status

- Any -
- Any -
- Draft
- Needs Approval
- Approved
- Published
- Tombstoned

# Add metadata

## Edit Metadata Test Donut Dataset

Required fields are marked with an asterisk (\*).

### Upload Files

Use Globus to upload your dataset files to the designated storage location.

1. Click **Upload with Globus** below. You will be taken to the Globus website.
2. Follow the prompts in Globus to authenticate and transfer your dataset files to the designated storage location.
3. Once your transfer is complete, return to this application.

[Upload with Globus](#)

DOI \*

10.13139/OLCF/3187457

Title \*

Enter a title for the dataset with enough detail to facilitate search and discovery.

Test Donut Dataset

### Author Information

**Author**

[Add one](#)

Sponsoring Organizations \*

Select the DOE Program Office(s) that funded the work for creating this dataset. Names of non-DOE funding organizations may be typed into this field. Separate multiple program offices with a semicolon and a space.

Office of Nuclear Energy (NE), Nuclear Infrastructure Programs

Originating Research Organization \*

Enter the name of the organization that performed the research or issued the dataset.

Oak Ridge National Laboratory (ORNL), Oak Ridge, TN (United States)

Other Contributing Organizations

Enter the name(s) of other organizations that provided funding or research resources for this dataset.

DOE Contract Number \*

Enter the DOE contract number(s) under which the work was funded. Separate multiple numbers with a semicolon and a space. When more than one number is entered, the first number is considered the primary number. The default value provided (AC05-00OR22725) is the DOE Prime Contract with UT-Battelle, LLC, for the management of ORNL.

DE-AC05-00OR22725

# Add authors

Author Information

**Author** —

First Name \*

Middle Name

Last Name \*

Author ORCID iD

Institutional Affiliation \*

Email \*

[Remove](#) [Move Up](#) [Move Down](#)

# Add related identifiers

Use related identifiers to point to:

- Preprints
- Accepted manuscripts
- Technical reports
- Input datasets
- Dataset versions or other locations
- Code repositories
- Software
- Instruments with DOIs

**Related Identifier Information**  
Add DOIs or URLs to related resources such as papers and other dataset versions.

**Related Identifier** —

**Related Identifier Type \***

**Relation Type \***  
Select a relationship between the dataset you are submitting and the DOI or URL you are referencing.

[Remove](#) [Move Up](#) [Move Down](#)

# Published landing page

constellation  
By Oak Ridge Leadership Computing Facility

Dataset Search FAQs Depositor Guide

Home > Dataset

View Edit Delete Revisions

## Data for "Understanding multiscale disorder in superconducting nanowire single photon detectors"

Nirjhar Sarkar | Oak Ridge National Laboratory

Download Dataset on Globus

### Description

This dataset addresses DC transport, dark-count measurements, and bias-dependent microwave transmission spectroscopy of superconducting nanowire. This publication includes the raw and processed data to produce figures in the paper "Understanding multiscale disorder in superconducting nanowire single photon detectors" (Sarkar et al., 2026).

### Funding Information

DOE Contract Number	AC05-00OR22725
Originating Research Organization	Oak Ridge National Laboratory (ORNL), Oak Ridge, TN (United States)
Sponsoring Organization	Office of Science (SC), Basic Energy Sciences (BES), Materials Sciences & Engineering Division (MSE)

### Related Works

- IsSupplementTo (DOI): <https://doi.org/10.48550/arXiv.2601.23277>

### Details

DOI  
<https://doi.org/10.13139/ORNLNCCS/3027645>

Release Date  
April 20, 2026

### Dataset

Dataset Type  
ND Numeric Data

### Cite This Dataset:

Sarkar, N. (2026). Data for "Understanding multiscale disorder in superconducting nanowire single photon detectors". Oak Ridge National Laboratory.  
<https://doi.org/10.13139/ORNLNCCS/3027645>.

### Acknowledgements

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