

National Data Service

**TOWARDS  
AN ARCHITECTURE  
FOR NATIONAL DATA SERVICES**

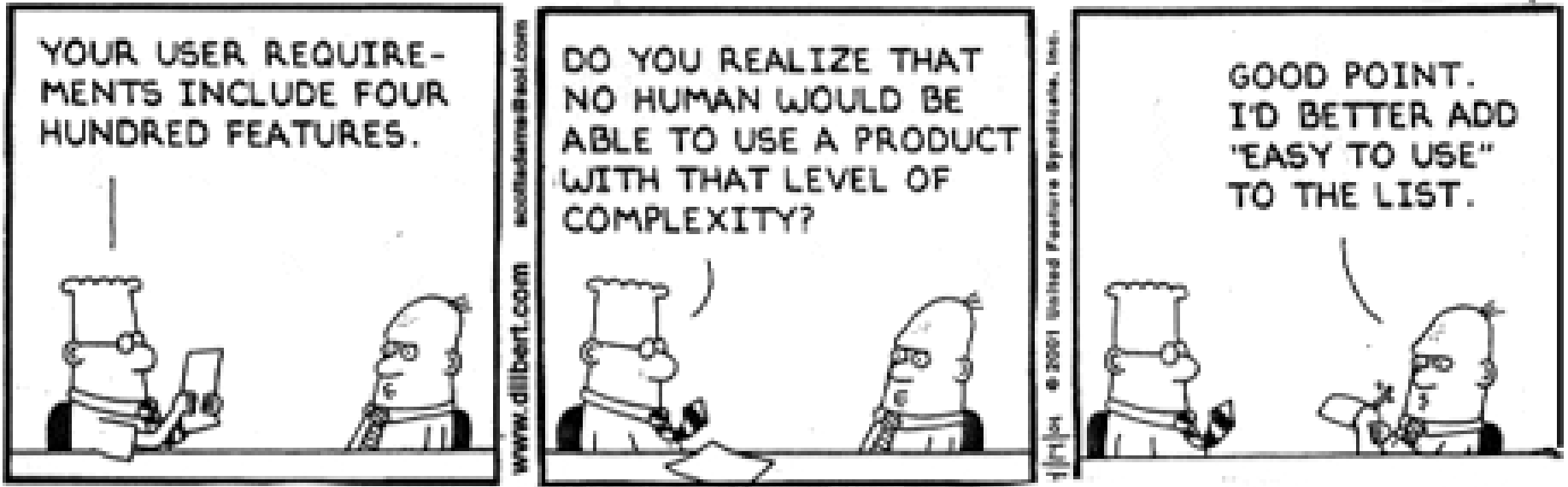
Ian Foster

Director, Computation Institute  
Argonne National Laboratory  
& The University of Chicago

@ianfoster

ianfoster.org

# Architecture?



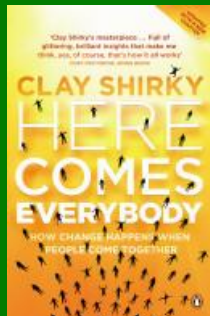
# Principle 1: Reduce data friction



Make simple things easy

Make hard things possible

For example,  
**publish-  
then-filter**



For example,  
cloud-hosted  
**software-as-a-service**

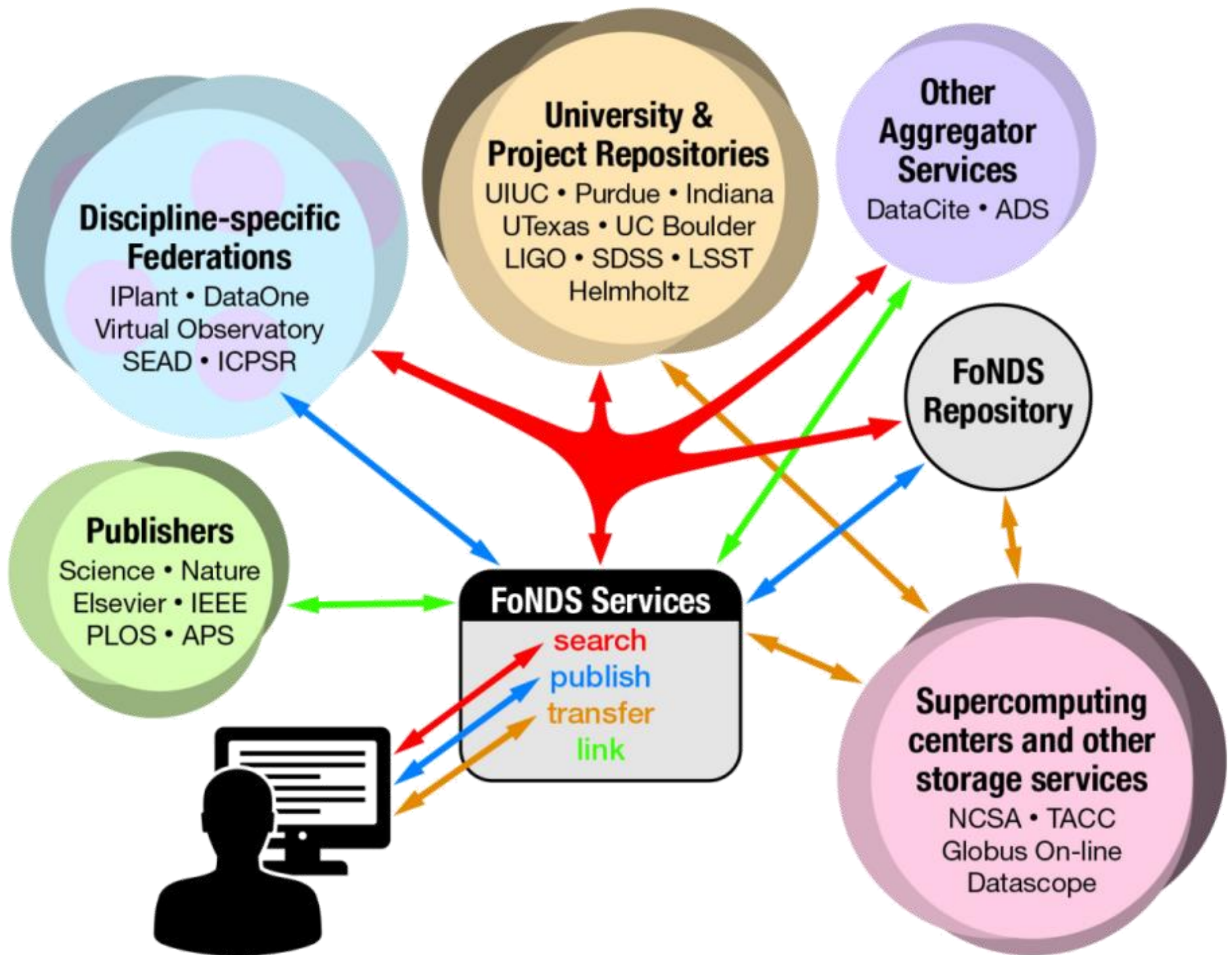


# Principle 2:

Small pieces, loosely joined

- Storage systems
- Content management
- Analysis systems
- Registries
- Identity management
- Data movers
- ... and many more ...

- REST interfaces
- Open
- Simple
- Composable
- Extensible
- Versioned



# Principle 3: Insist on stories

- For example:
  - “I need to store/backup/archive my data”
  - “I need to transfer/mirror my data”
  - “I need to share my data”
  - “I need to publish my data”
  - “I need to discover published data”
  - “I need to analyze my data”
- Good stories are detailed, urgent, popular

# We have much to build on and/or integrate with

- Agave
- Brown Dog
- DataCite
- DATAone
- Dataverse
- Earth System Grid
- Globus
- Globus Connect
- InCommon
- iPlant
- ORCID
- SEAD
- XSEDE
- Zenodo
- Many more
- Many many more!

# Globus demonstration

**Globus** cloud-hosted software-as-a-service for:

- Data transfer, sync, and sharing
- Identity and group management
- Data publication and discovery

**Globus Connect** software to integrate resources and institutions



# What does it mean to **publish**?

*Data is:*

Identified

Described

Curated

Verifiable

Accessible

Preserved

# What does it mean to **discover**?

*I can:*

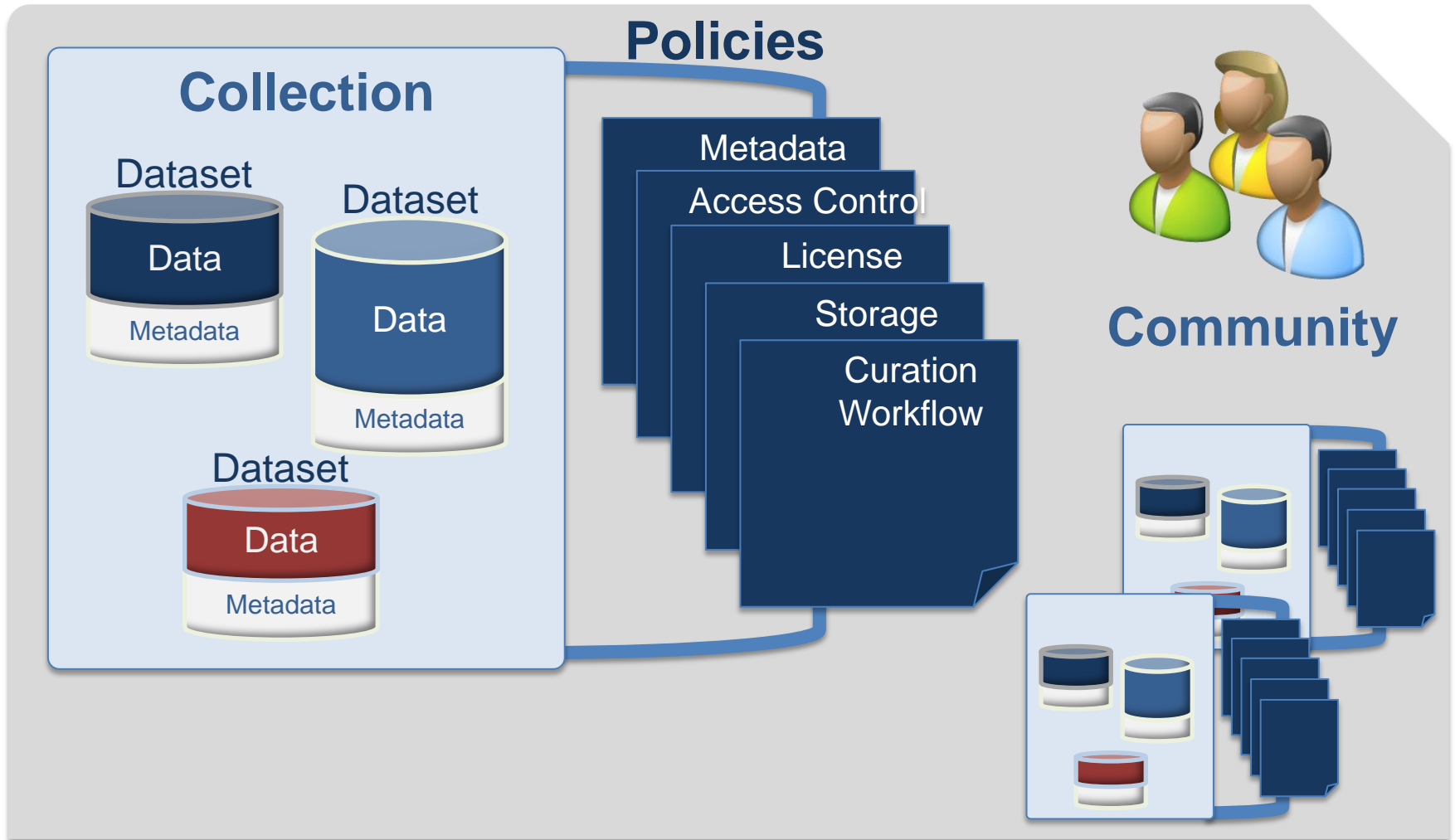
Search

Browse

Access

*the data*

# Data publication and discovery



# Takeaway messages

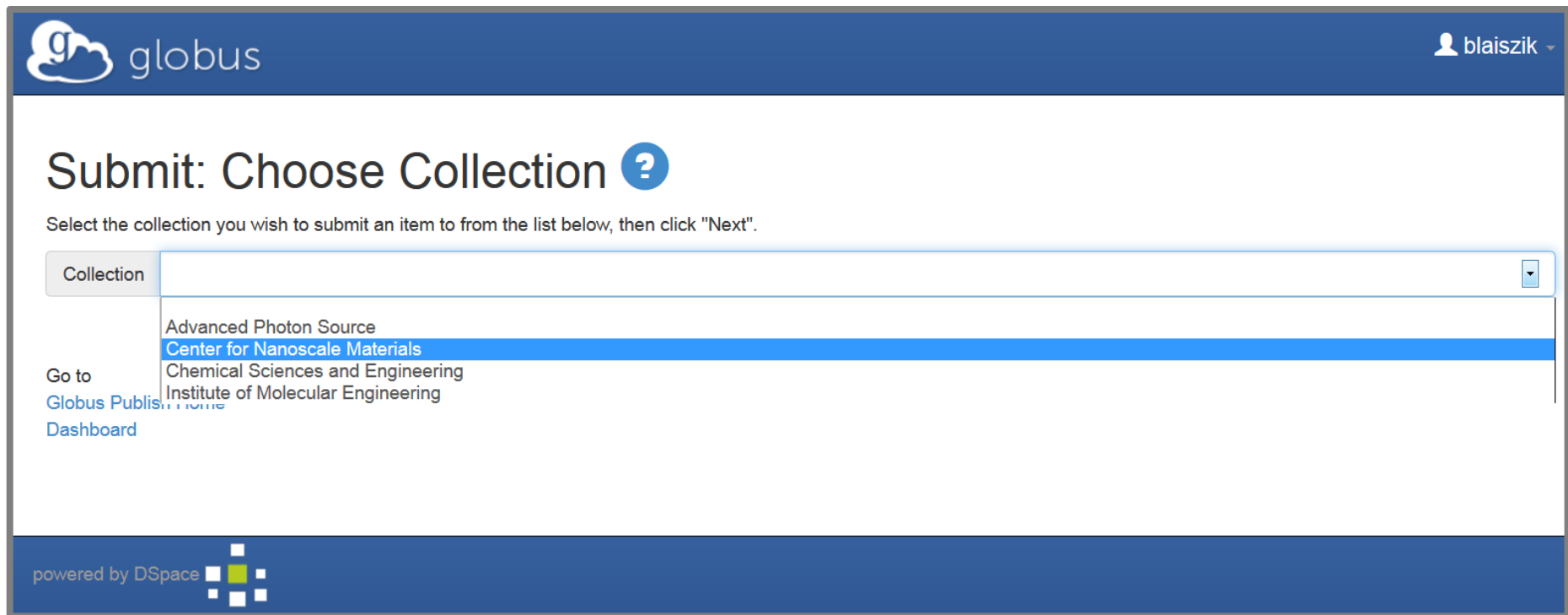
- Three principles:
  - Reduce data friction
  - Small pieces, loosely joined
  - Insist on stories
- We have strong components to start with
- We'd like from you:
  - Stories to inform and prioritize
  - Volunteers to deploy and explore

**The following are backup slides  
in case network failure prevents  
the live demonstration**

# Publish dashboard

The screenshot shows the Globus Publish dashboard interface. At the top left is the Globus logo, and at the top right are navigation links for Search, Publish, Manage Data, Groups, Support, and a user profile for blaiszik. Below the navigation bar is a blue header bar with the text "Globus". Underneath is another blue bar labeled "Dashboard: Ben Blaiszik" with a help icon. The main content area contains two buttons: "Start a New Submission" (green) and "View Accepted Submissions" (blue). At the bottom left, it says "powered by DSpace" with the DSpace logo.

# Start a new submission



The screenshot shows the 'Submit: Choose Collection' page in the Globus interface. The page header includes the Globus logo and the user name 'blaiszik'. The main heading is 'Submit: Choose Collection' with a help icon. Below the heading is a instruction: 'Select the collection you wish to submit an item to from the list below, then click "Next".' A dropdown menu is open, showing a list of collections: 'Advanced Photon Source', 'Center for Nanoscale Materials' (highlighted), 'Chemical Sciences and Engineering', and 'Institute of Molecular Engineering'. On the left side of the dropdown, there are navigation links: 'Go to', 'Globus Publications Home', and 'Dashboard'. The footer of the page indicates it is 'powered by DSpace' with the DSpace logo.

globus blaiszik

## Submit: Choose Collection ?

Select the collection you wish to submit an item to from the list below, then click "Next".

Collection

- Advanced Photon Source
- Center for Nanoscale Materials**
- Chemical Sciences and Engineering
- Institute of Molecular Engineering

Go to  
Globus Publications Home  
Dashboard

powered by DSpace





# Submit: Describe this Item ?

Please fill further information about this submission below.

Enter appropriate subject keywords or phrases below.

**Subject Keywords**

self-healing	Remove Entry	circuit	Remove Entry
microcapsules	Remove Entry		Add More

Enter the names of any sponsors and/or funding codes in the box below.

**Sponsors**

This material is based upon work supported as part of the Center for Electrical Energy Storage - Tailored Interfaces, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number (919 DOE ANL 9F-31921 NS).

Enter a description for this item in the box below.

**Description**

Thermomechanical failure of conductive pathways in highly integrated circuits results in loss of function that is often impossible to repair and remains a long-standing problem hindering advanced electronic packaging. Prior approaches to restoration of conductivity rely on external intervention in the form of heating or manual delivery of relatively low conductivity materials. Here, we demonstrate autonomic healing of an electrical circuit with nearly full recovery of conductance (ca. 99%) less than one millisecond after damage. The rapid restorative

Enter the name of experiment for this item below.

**Experiment**

Enter the names of materials used in this experiment below.

**Material**

Gallium	Remove Entry	Gold	Remove Entry
Indium		circuitboard	Add More

Enter the energy density used in this experiment.

**Energy Density (mAh/g)**

Enter the Argonne GUP that this experiment was conducted under.

**GUP**

Describe submission:  
2) Science metadata

# Assemble the dataset

The screenshot shows the Globus user interface for the 'Submit: Assemble a dataset' workflow. At the top, the Globus logo and the user name 'blaiszik' are visible. Below the logo is a navigation bar with buttons for 'Describe', 'Upload', 'Verify', 'License', and 'Complete'. The 'Submit: Assemble a dataset' title is followed by a help icon. The main text explains that a unique endpoint will be created for asynchronous dataset assembly. A green 'Select Files' button is centered on the page. At the bottom, a navigation bar contains buttons for '< Previous', 'Cancel/Save', 'Skip dataset assembly >', and 'Next >'. The footer includes the 'powered by DSpace' logo.

# Transfer Files

Get Globus Connect Personal

Turn your computer into an endpoint.

Endpoint:  Go

Path:  Go

File Name	Size
20130311-Conductivity-SH-original-4.txt	92 kB
20130317-capsule-sizing-4.csv	6 kB
20130324-Healed-fracture-tomo-2.csv	93 kB
20130328-capsule-sizing-1.txt	45 kB
20130514-Conductivity-SH-healed-3.tif	72 kB
20130516-Healed-fracture-tomo-4.tif	80 kB
20130517-Gain-capsule-SEM-1.png	99 kB
20130517-Gain-capsule-SEM-4.xlsx	38 kB
20130518-Conductivity-SH-healed-4.csv	30 kB
20130519-Gain-capsule-SEM-3.tif	53 kB
20130523-Conductivity-SH-original-1.csv	91 kB
20130524-Gain-capsule-SEM-2.csv	68 kB
20130611-Conductivity-SH-healed-2.xlsx	22 kB
20130621-Healed-fracture-tomo-1.csv	89 kB
20130622-Conductivity-SH-original-3.tif	36 kB
20130714-Conductivity-SH-original-2.tif	22 kB
20130729-Conductivity-SH-healed-1.txt	69 kB
20130813-capsule-sizing-3.tif	44 kB
20130828-Healed-fracture-tomo-3.txt	85 kB
20130925-capsule-sizing-2.tif	41 kB

more options    Label This Transfer  This will be displayed in your transfer activity

Endpoint:  Go

Path:  Go

File Name	Size
20130311-Conductivity-SH-original-4.txt	92 kB
20130317-capsule-sizing-4.csv	6 kB
20130324-Healed-fracture-tomo-2.csv	93 kB
20130328-capsule-sizing-1.txt	45 kB
20130514-Conductivity-SH-healed-3.tif	72 kB
20130516-Healed-fracture-tomo-4.tif	80 kB
20130517-Gain-capsule-SEM-1.png	99 kB
20130517-Gain-capsule-SEM-4.xlsx	38 kB
20130518-Conductivity-SH-healed-4.csv	30 kB
20130519-Gain-capsule-SEM-3.tif	53 kB
20130611-Conductivity-SH-healed-2.xlsx	22 kB
20130621-Healed-fracture-tomo-1.csv	89 kB
20130622-Conductivity-SH-original-3.tif	36 kB

Transfer files to submission endpoint

## Activity



publish#publish-server to publish#submission\_11  
transfer completed a few seconds ago



# Submit: Dataset Assembled Successfully

Your dataset was successfully assembled.

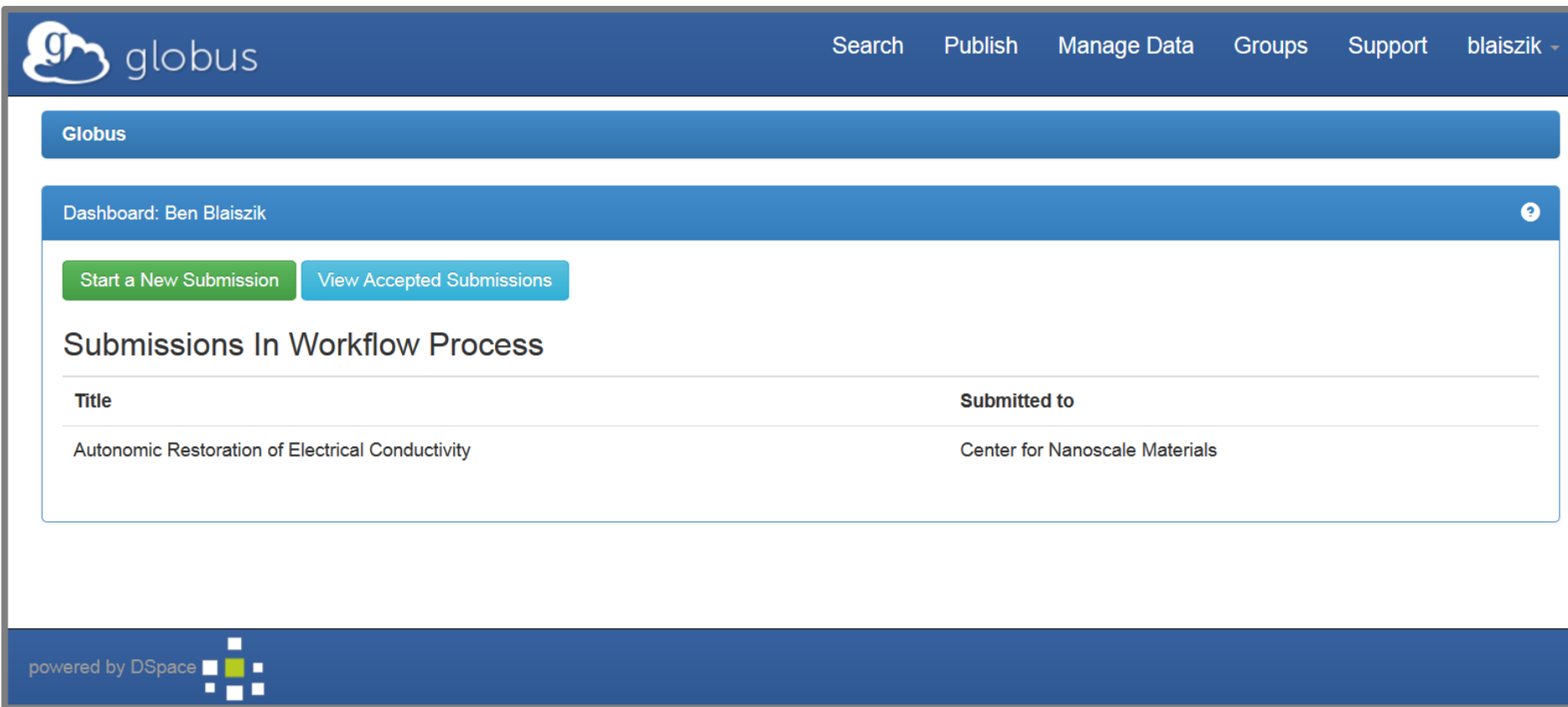
The table below shows the files which are included in this item.

Primary bitstream	File		Size	Description	File Format	
<input type="radio"/>	<a href="#">20130311-Conductivity-SH-original-4.txt</a>	Remove	94208 bytes	None  Change	Text (known)	Change
<input type="radio"/>	<a href="#">20130317-capsule-sizing-4.csv</a>	Remove	6144 bytes	None  Change	Unknown (unsupported)	Change
<input type="radio"/>	<a href="#">20130324-Healed-fracture-tomo-2.csv</a>	Remove	95232 bytes	None  Change	Unknown (unsupported)	Change
<input type="radio"/>	<a href="#">20130328-capsule-sizing-1.txt</a>	Remove	46080 bytes	None  Change	Text (known)	Change
<input type="radio"/>	<a href="#">20130514-Conductivity-SH-healed-3.tif</a>	Remove	73728 bytes	None  Change	TIFF (known)	Change
<input type="radio"/>	<a href="#">20130516-Healed-fracture-tomo-4.tif</a>	Remove	81920 bytes	None  Change	TIFF (known)	Change
<input type="radio"/>	<a href="#">20130517-Gain-capsule-SEM-1.png</a>	Remove	101376 bytes	None  Change	image/png (known)	Change
<input type="radio"/>	<a href="#">20130517-Gain-capsule-SEM-4.xlsx</a>	Remove	38912 bytes	None  Change	Microsoft Excel XML (known)	Change
<input type="radio"/>	<a href="#">20130518-Conductivity-SH-healed-4.csv</a>	Remove	30720 bytes	None  Change	Unknown (unsupported)	Change
<input type="radio"/>	<a href="#">20130519-Gain-capsule-SEM-3.tif</a>	Remove	54272 bytes	None  Change	TIFF (known)	Change
<input type="radio"/>	<a href="#">20130611-Conductivity-SH-healed-2.xlsx</a>	Remove	22528 bytes	None  Change	Microsoft Excel XML (known)	Change
<input type="radio"/>	<a href="#">20130621-Healed-fracture-tomo-1.csv</a>	Remove	91136 bytes	None  Change	Unknown (unsupported)	Change
<input type="radio"/>	<a href="#">20130622-Conductivity-SH-original-3.tif</a>	Remove	36864 bytes	None  Change	TIFF (known)	Change

Add Another File

Check dataset is assembled correctly

# Submission now in curation workflow



The screenshot shows the Globus user interface. At the top left is the Globus logo. The top navigation bar includes links for Search, Publish, Manage Data, Groups, Support, and a user profile for blaiszik. Below the navigation bar is a blue header with the text "Globus". The main content area is titled "Dashboard: Ben Blaiszik" and contains two buttons: "Start a New Submission" (green) and "View Accepted Submissions" (blue). Below these buttons is a section titled "Submissions In Workflow Process" which contains a table with one row of submission data.

Title	Submitted to
Autonomic Restoration of Electrical Conductivity	Center for Nanoscale Materials

powered by DSpace

# Search published datasets



globus

Search Publish Manage Data Groups Support

## Discover Data

energy\_density | num\_samples | protocol\_version | 2000

Refine Search All Endpoints Collections

\*

Transfer Tag Analyze

Start Destination: Home (blaiszik#laptop/) | SNS (go#ep2/home/SNS)  
New Destination

All None Inverse

7 results found | > 0.0 B

0 selected | > 0.0 B

### TiO<sub>2</sub>-luciferase Nanoconjugates for Enhanced Photodynamic Therapy

Blaiszik, Ben; Rajh, Tijana;

Photodynamic therapy (PDT) is an emergent technology used for the treatment of cancers, psoriasis, and other autoimmune diseases.<sup>1</sup> In this method, light energy is converted to chemical energy, creating highly reactive oxygen species (ROS), which under appropriate conditions are highly disruptive for cell metabolism and lead to cell death. PDT critically depends on the possibility of delivering light in the vicinity of the tumor. At present the small penetration depth of light in the body is the primary limitation of PDT, and the tumor has to be at most within 1 cm of the light source. This eliminates the possibility for treatment of tumors that are located deep in the tissues.

04/15/2014

9:51 PM

12 files

Center for Nanoscale Materials

[View Dataset](#)

TiO<sub>2</sub> nanoconjugates photodynamic

sample\_id:1 protocol\_version:7

### Detection and role of trace impurities in high-performance organic solar cells

Nikiforov, Maxim; Lai, Barry; Chen, Wei; Schaller, Richard; Darling, Seth;

Trace impurities in organic solar cells, such as those from residual catalyst material in conjugated polymers, are often ignored but are known to deleteriously affect device performance. Batch-to-batch variations in the nature and quantity of such impurities leads to widespread issues with irreproducible optoelectronic function, yet to date no technique has emerged that is reliably capable of identifying the character of impurities or their concentration in organic photovoltaic active layer blends. Here we focus on state-of-the-art, high-performance bulk heterojunction blends and show that synchrotron-based X-ray fluorescence can detect and quantify trace concentrations of metal impurities in these systems.

04/15/2014

10:04 PM

13 files

Center for Nanoscale Materials

[View Dataset](#)

solar impurities x-ray fluorescence organic solar cells

num\_samples:7 protocol\_version:2

# Search across collections



globus

Search Publish Manage Data Groups Support

## Discover Data

energy\_density | num\_samples | protocol\_version | 2000

Refine Search All Endpoints Collections

Li-ion autonomic



Transfer

Tag

Analyze

Start

Destination: Home (blaiszik#laptop/) | SNS (go#ep2/home/SNS)

New Destination

All None Inverse

8 results found | > 0.0 B

0 selected | > 0.0 B

### Autonomic Shutdown of Lithium-Ion Batteries Using Thermo-responsive Microspheres

Baginska, Marta; Blaiszik, Ben; Sottos, Nancy; White, Scott;

Autonomic, thermally-induced shutdown of Lithium-ion (Li-ion) batteries is demonstrated by incorporating thermo-responsive polymer microspheres (ca. 4  $\mu\text{m}$ ) onto battery anodes or separators. When the internal battery environment reaches a critical temperature, the microspheres melt and coat the anode/separator with a nonconductive barrier, halting Li-ion transport and shutting down the cell permanently. Scanning electron microscopy images of electrode surfaces from cells that have undergone autonomic shutdown provides evidence of melting, wetting, and resolidification of PE into the anode and polymer film formation at the anode/separator interface.

Li-ion battery safety autonomic shutdown

energy\_density:250 num\_samples:15

04/15/2014

9:20 PM

16 files

Chemical Sciences and Engineering

View Dataset

### Synthesis, Characterization, and Structural Modeling of High-Capacity, Dual Functioning MnO<sub>2</sub> Electrode/Electrocatalysts for Li-O<sub>2</sub> Cells

Trahey, Lynn; Chan, Maria; Blaiszik, Ben;

It has become clear that cycling lithium-oxygen cells in carbonate electrolytes is impractical, as electrolyte decomposition, triggered by oxygen reduction products, dominates the cell chemistry. This research shows that employing an  $\alpha$ -MnO<sub>2</sub>/ramsdellite-MnO<sub>2</sub>electrode/electrocatalyst results in the formation of lithium-oxide-like discharge products in propylene carbonate, which has been reported to be extremely susceptible to decomposition. X-ray photoelectron data have shown that what are likely lithium oxides (Li<sub>2</sub>O<sub>2</sub> and Li<sub>2</sub>O) appear to form and decompose on the air electrode surface, particularly at the MnO<sub>2</sub> surface, while Li<sub>2</sub>CO<sub>3</sub> is also formed.

Li-ion Li-air manganese

energy\_density:2500

04/16/2014

9:56 AM

4 files

Center for Nanoscale Materials

View Dataset

# Discover a published dataset

## Discover Data

energy\_density | num\_samples | protocol\_version | 2000

Refine Search All Endpoints Collections

energy\_density>1500 microcapsules

Transfer

Tag

Analyze

Start

Destination: Home (blaiszik#laptop/) | SNS (go#ep2/home/SNS)

New Destination

All None Inverse

3 results found | > 0.0 B

0 selected | > 0.0 B

### Autonomic Restoration of Electrical Conductivity

Blaiszik, Ben; Kramer, Charlotte; Grady, Martha; Sottos, Nancy; White, Scott;

Thermomechanical failure of conductive pathways in highly integrated circuits results in loss of function that is often impossible to repair and remains a long-standing problem hindering advanced electronic packaging. Prior approaches to restoration of conductivity rely on external intervention in the form of heating or manual delivery of relatively low conductivity materials. Here, we demonstrate autonomic healing of an electrical circuit with nearly full recovery of conductance (ca. 99%) less than one millisecond after damage. The rapid restorative mechanism relies on the triggered release and transport of microencapsulated eutectic gallium–indium (Ga–In) liquid metal into the broken conductive pathway. For a relatively small volume fraction of microcapsules that are patterned on gold (Au) lines, all of the damaged circuits heal with high efficiency. This autonomic healing system shows the potential for more sustainable electronic devices with increased fault-tolerance, improved circuit reliability, and extended service life.

04/21/2014

2:26 PM

13 files

Center for Nanoscale Materials

View Dataset

self-healing circuit microcapsules

energy\_density:2000

### Synthesis, Characterization, and Structural Modeling of High-Capacity, Dual Functioning MnO<sub>2</sub> Electrode/Electrocatalysts for Li-O<sub>2</sub> Cells

Trahey, Lynn; Chan, Maria; Blaiszik, Ben;

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04/16/2014

9:56 AM

4 files

Center for Nanoscale Materials

View Dataset

Li-ion Li-air manganese

energy\_density:2500



# Select a published dataset



globus

Search Publish Manage Data Groups Support

## Discover Data

energy\_density | num\_samples | protocol\_version | 2000

Refine Search All Endpoints Collections

energy\_density>1500 microcapsules



Transfer

Tag

Analyze

Start

Destination: Home (blaiszik#laptop/) | SNS (go#ep2/home/SNS)

New Destination

All None Inverse

3 results found | > 0.0 B

0 selected | > 0.0 B

### Autonomic Restoration of Electrical Conductivity

Blaiszik, Ben; Kramer, Sharlotte; Grady, Martha; Sottos, Nancy; White, Scott;

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04/21/2014

2:26 PM

13 files

Center for Nanoscale Materials

View Dataset

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04/16/2014

9:56 AM

4 files

Center for Nanoscale Materials

View Dataset

Li-ion Li-air manganese

energy\_density:2500

# View downloaded dataset

The screenshot displays a Mac OS file explorer window titled "SynthesisData" containing the following files:

Name	Date Modified	Size	Kind
20120101 - Atomic-configurations.png	Today 2:45 PM	1.2 MB	Portab...image
20120108 - Cycling.png	Today 2:45 PM	1.6 MB	Portab...image
20120110 - Lithiation.jpeg	Today 2:45 PM	135 KB	JPEG image
20120201 - Overview.png	Today 2:45 PM	617 KB	Portab...image

Below the file explorer, three windows are visible:

- 20120108 - Cycling.png:** A scanning electron microscope (SEM) image showing a dense network of thin, needle-like structures. A scale bar at the bottom indicates 10 μm.
- 20120110 - Lithiation.jpeg:** A 3D molecular model showing a structure composed of green and blue spheres. The spheres are arranged in a layered, interconnected pattern. Labels "Li" and "Si" are present, indicating the presence of Lithium and Silicon atoms.
- 20120108 - Cycling.png (larger view):** A larger SEM image of the same material, showing a dense, interconnected network of thin, needle-like structures. A scale bar at the bottom indicates 10 μm.