Materials Data Facility as Community Database to Share Nano-manufacturing Recipes

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Build data services to

• **Empower researchers to publish data, regardless of size, type, and location**

• **Automate data and metadata extraction and ingest**

• **Enable unified search and discovery across disparate materials data sources**

Deploy with APIs to simplify connection to other data efforts and to enable automation
The Materials Data Facility (MDF) is an effort to build a set of data services to support materials science researchers. MDF offers a data publication service where materials scientists can publish, discover, preserve, and share research datasets ranging in size from kilobytes to terabytes.
Materials Data Facility Processes

- **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
- Currently holds ~30TB of data from over 150 authors, millions of individual results
Gr-ResQ
Graphene Recipes for Synthesis of High Quality Materials

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Graphene

2-dimensional sheet of carbon atoms
“Honeycomb” lattice

Properties
• High strength
• Electrically conductive
• Lightweight
• Flexible

Applications
• Transparent conductor
• Flexible electronics
• Mechanical composites

https://www.nature.com/news/graphene-the-quest-for-supercarbon-1.14193
How Do We Make It?

1) diffusion of precursors
2) adsorption on the surface
3) chemical reaction
4) desorption of adsorbed material
5) diffusion of byproducts

main stream of reaction gases

boundary layer
interface
substrate

surface diffusion

http://www.plasma-electronics.com/chemical-vapor-deposition.html
CVD Recipes

Over 200 variables per sample

- Furnace temperature
- Furnace pressure
- Gas flow
- Sample position
- Annealing condition
- Growing condition
- Cooling condition
- Sample preparation
- Catalyst
- Furnace dimensions
Challenges With CVD

- Poor repeatability of experiments
- Lack of quantitative description of the parameter space
- Necessity for centralized database of existing experimental data
Publication to MDF

• We treat each recipe as a dataset
• Subsequent analyses are also datasets
• Collections of datasets can be bundled together with a single, DOI minted for publication
• Datasets are searchable via Forge