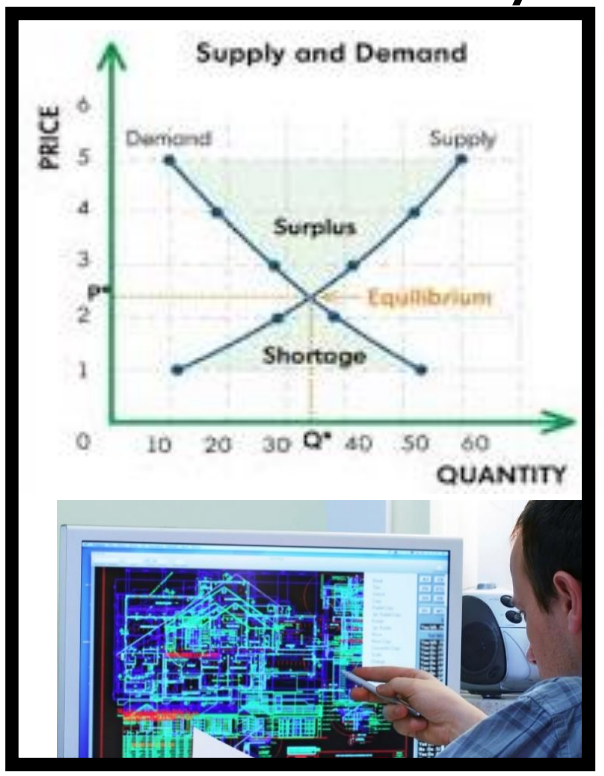
# NETL's Intramural Research Program in Advanced Coal Processing

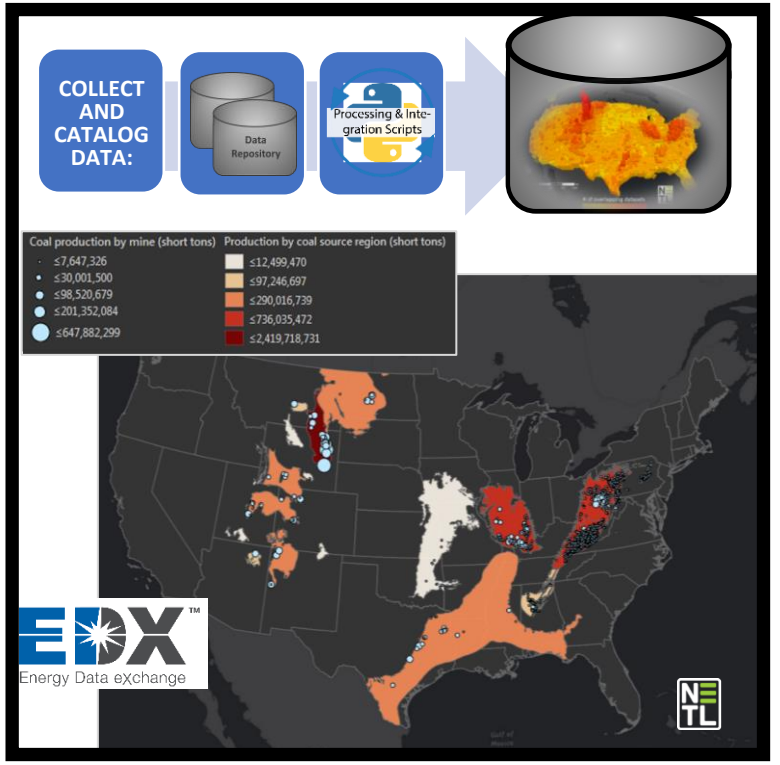
**Christopher Matranga**, *Materials Engineering & Manufacturing Division*

## Materials Discovery & Design

## Market, Process, & Environmental Analysis




## American Coal Database



# Outline:

- **Materials Discovery & Design**
- Market, Process, & Environmental Analysis
- American Coal Database

# Materials Discovery & Design

NATIONAL ENERGY TECHNOLOGY LABORATORY

Coal Value Chain →

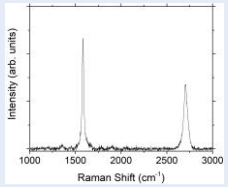
**Domestic Feedstocks** | **Carbon Materials** | **Commercial Applications**

## Domestic Feedstocks

### Coal, Char, Pitch, Liquids

## Carbon Materials

### Low Defect Graphene Films

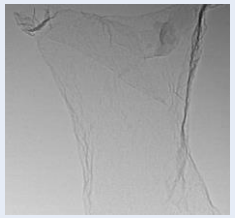



### Graphene Nanoflake

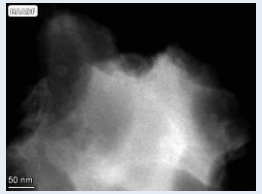
### Graphite

### Graphene Quantum Dots

### Carbon Nanosheets



### Porous Carbons



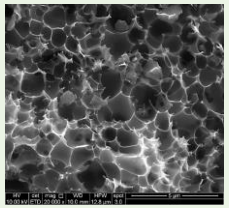
## Commercial Applications

### Biosensing & Medical Diagnostics

### Carbon Electronics

### Construction Materials

### Energy Storage (Gas & Electrical)



# Manufacturing Graphite from Domestic Coal and Coal/Biomass Blends

NATIONAL ENERGY TECHNOLOGY LABORATORY

**NEW START April 2021**

## NETL Approach:

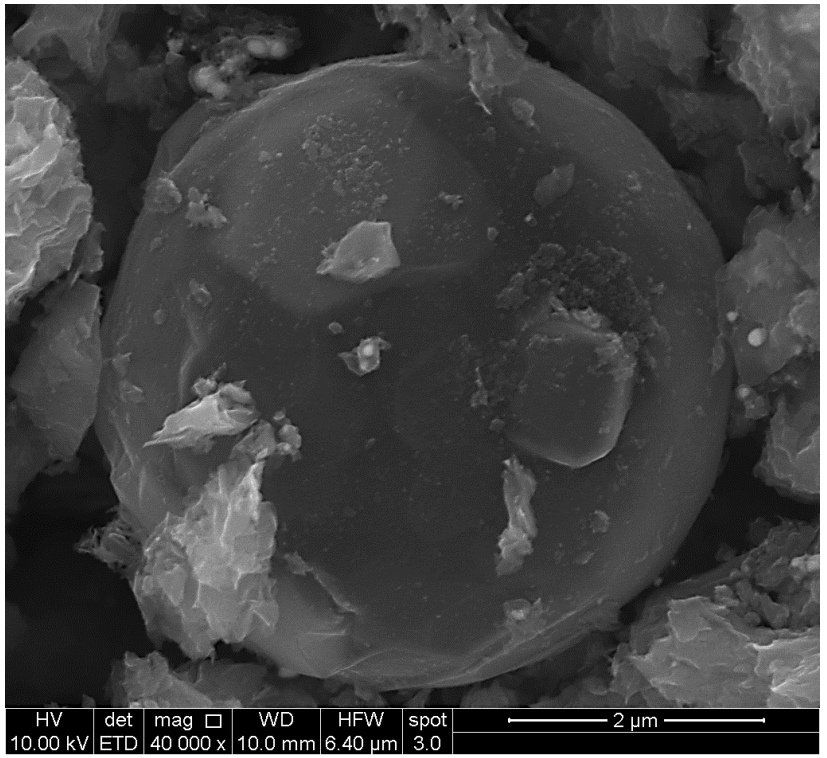
**Improving Graphite Manufacturing**

- **Reduce environmental footprint:** w/catalytic & microwave processes to reduce manufacturing temp & time
- **Lower manufacturing costs:** polygeneration of graphite + other carbon products w/low-cost feedstocks

**Economic & Environmental Analysis of Graphite Manufacturing**

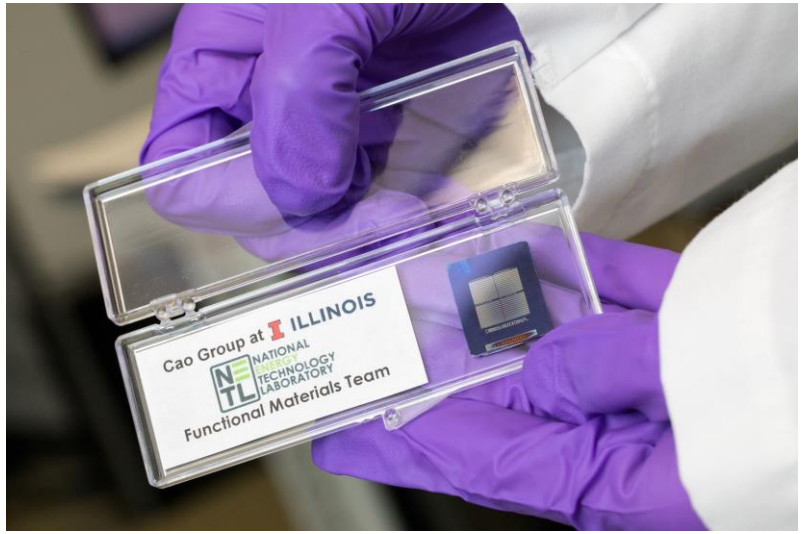
- **Estimate market penetration** for coal/biomass utilization
- **Quantify impact on jobs** in mining & manufacturing
- **Analyze GHG & environmental footprint** of coal/biomass utilization for graphite

**NETL's Low Temp Graphitization of Coal**

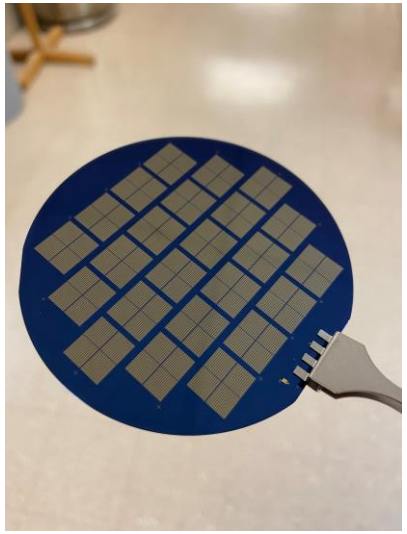


# Carbon Electronics: Memristor Computer Memory

**1-inch prototype (~1000 Devices)**




**3-inch prototype (~24,000 Devices)**



**Coal-based Memristor Devices:**

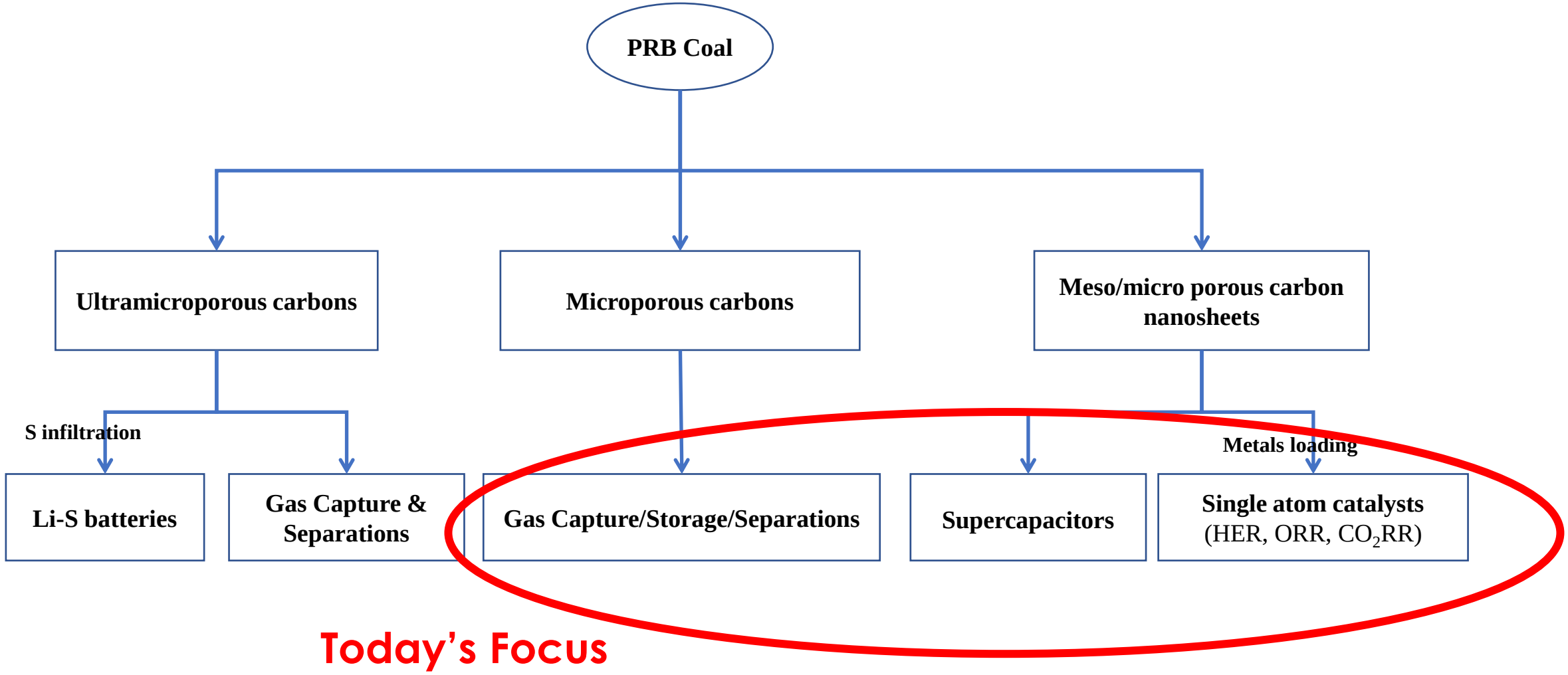
- Made from char waste of pilot scale coal to liquids process (Carbon Technology Company, VA)
- Atomically thin amorphous film of carbon used as dielectric switching medium
- Lowers energy consumption 10-100 X
- Improves device performance (filament formation/retraction)
- Material is stable during fabrication & long-term device operation
- Stable operation for 1000s+ of cycles
- **Patent Filed 3/2021**
- **License being negotiated w/industrial partner**

ILLINOIS
UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN

**Prof Qing Cao**
**Dept Materials Science**

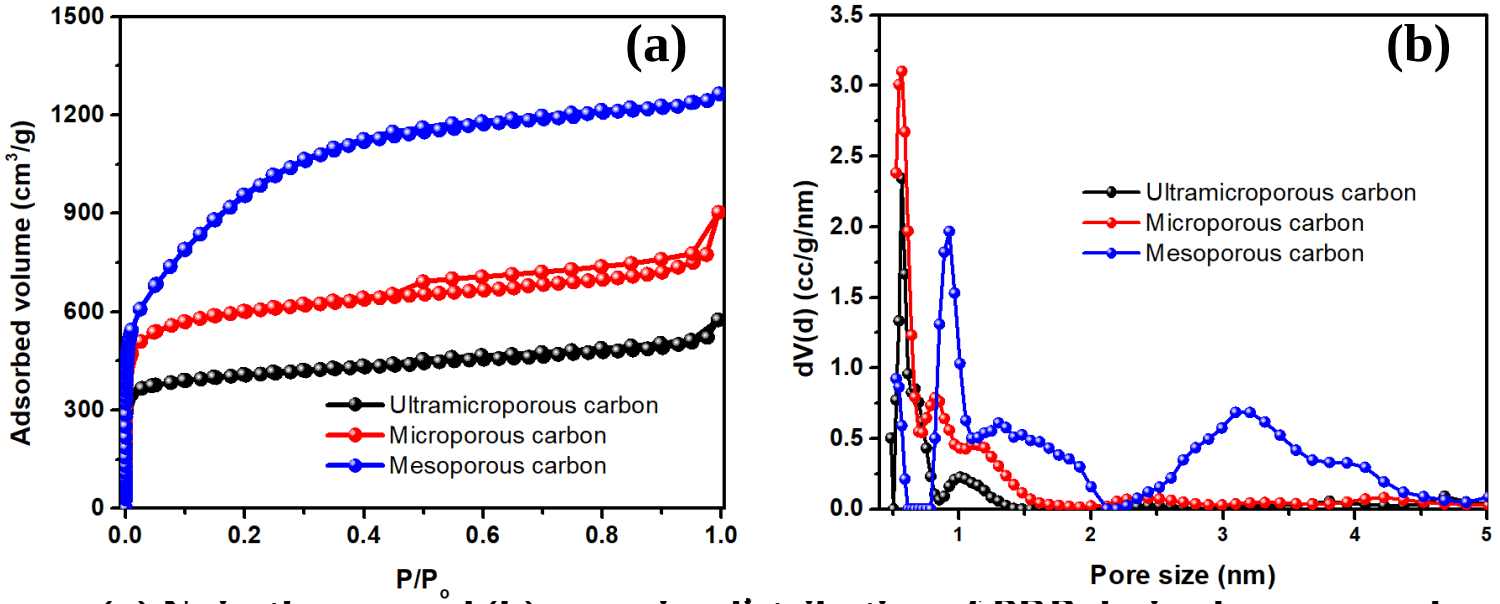
**Materials Engineering & Manufacturing Division**

# Tunable Porous Carbon Materials From Powder River Basin Coal




**Today's Focus**

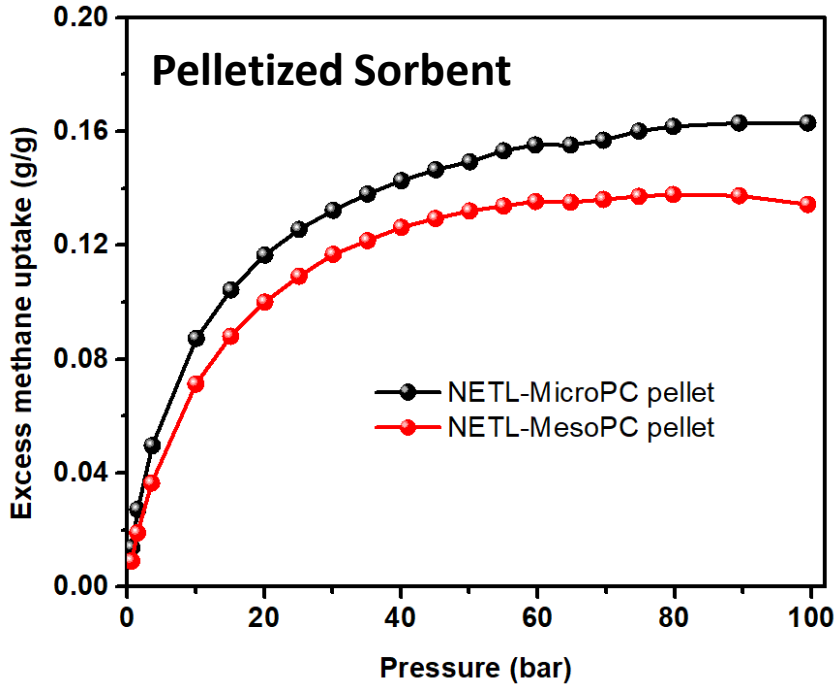
# Tunable Pore Sizes, Highly Microporous



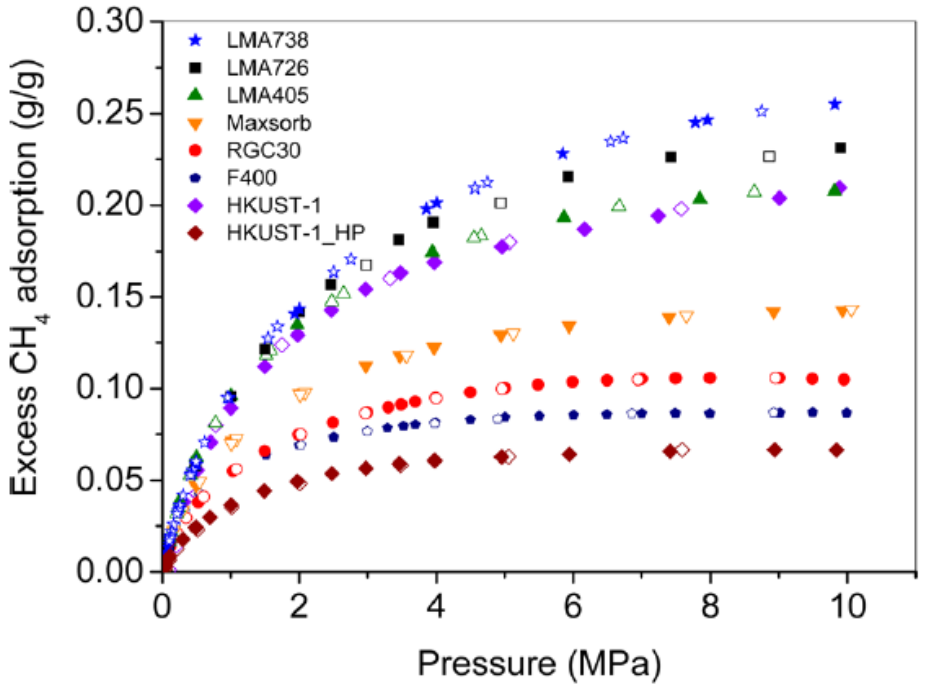

**(a) $N_2$ isotherms and (b) pore size distribution of PRB derived porous carbons**

| | BET SSA ($m^2/g$) | QSDFT SSA ($m^2/g$) | Ultramicropore volume (≤ 0.7 nm; $cm^3/g$)*† | Micropore volume (≤ 2.0 nm; $cm^3/g$)*† | Mesopore volume (2.0 – 50.0 nm; $cm^3/g$)*† | Total pore volume ($cm^3/g$)* |
|---|---|---|---|---|---|---|
| **Ultramicroporous carbon** | **1480** | **2120** | **0.42** (55.3%) | **0.62** (81.6%) | **0.14** (18.4%) | **0.76** |
| **Microporous carbon** | **2250** | **2440** | **0.41** (37.3%) | **0.81** (73.6%) | **0.29** (26.4%) | **1.1** |
| **Mesoporous carbon** | **3500** | **2760** | **0.10** (5.6 %) | **0.85** (47.2%) | **0.95** (52.8%) | **1.8** |

# Porous carbons for methane storage

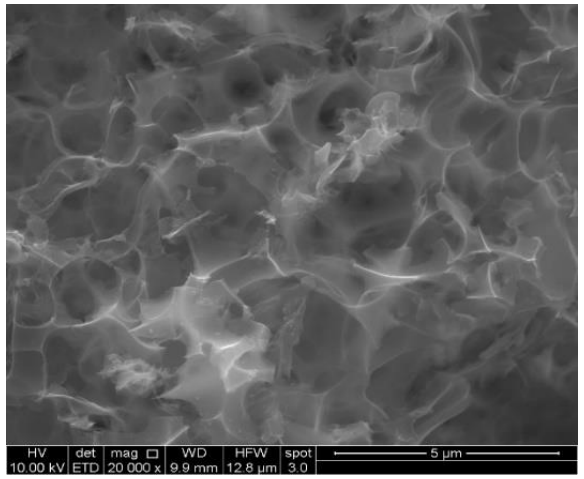



**Methane uptake of PRB derived porous carbons at 25 °C, 100 bar,**

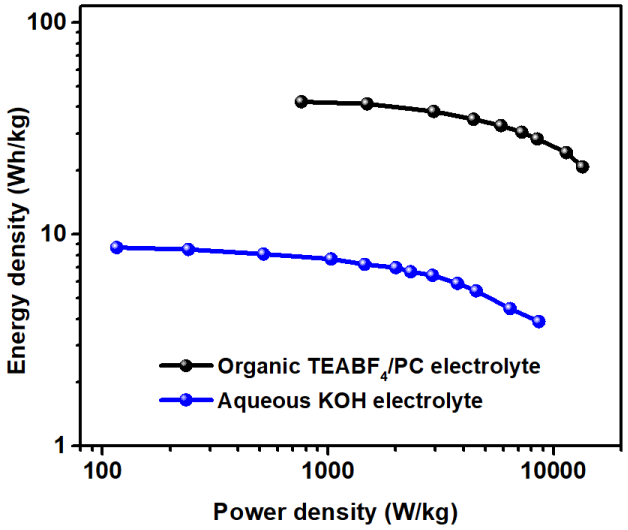



**Chem. Mater. 2015, 27, 3, 959–964**

# Porous carbon nanosheets (CNSs) for supercapacitors




SEM image of coal derived CNS




Ragon plots of CNS supercapacitors

**Comparison of carbon-based supercapacitors, 6M KOH electrolyte, two-electrode cell**

| | Capacitance at 1.0 A/g | Rate capacity (1.0 to 20 A/g) | Cycling stability | Reference |
|---|---|---|---|---|
| NETL CNS | 240 F/g | 80 % | >90 %, 100,000 cycles, 4 A/g | NETL |
| N-doped graphene | 250 F/g | 76 % | 95 %, 10,000 cycles, 2 A/g | Nano Lett., 2011, 11, 2472–2477 |
| Holey graphene hydrogel | 310 F/g | 88 % | 95 %, 20,000 cycles, 25 A/g | Nat. Commun., 2014, 5, 4554 |
| Immense surface area carbon | 280 F/g | 85 % | 80 %, 75,000 cycles, 25 A/g | J. Mater. Chem. A, 2017, 5, 13511 |
| Commercial AC Norit | 85 F/g | 80 % | Not reported | J. Mater. Chem. A, 2017, 5, 13511 |

**Performance in other solvent systems**

| | Capacitance (F/g) | Rate capacity | Cycling stability | Energy Density (Wh/kg) | Power Density (W/kg) | Voltage (V) | Solvent |
|---|---|---|---|---|---|---|---|
| NETL CNS | up to 200 | 55 % | >90 %, 30,000 cycles | 4.5-17.5 | 200-7,000 | 0-1.6 | 1 M $Na_2SO_4$ |
| NETL CNS | up to 145 | 70 % | T.B.D. | 20-42 | 700-14,000 | 0-3 | 1M $TEABF_4$ w/propylene carbonate |

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# Market Analysis

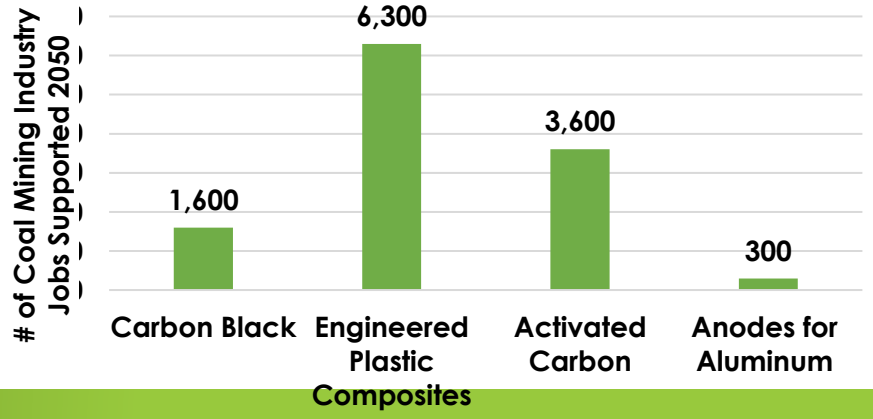
## Products

| EY 18 | EY 19 | | EY 20 |
|---|---|---|---|
| • Carbon Fiber | • Carbon Fiber Cement | • Conductive Inks | • Carbon Black |
| • Graphene | • Graphene Cement | • Carbon Foam | • Engineered Composites |
| | • Roofing Tiles | • Battery Anodes | • Activated Carbon |
| | • Carbon Composites | | • Al Anodes |

## Market Impact

| | U.S. Product Consumption (MMt) | U.S. Production of Carbon Product (MMt) | U.S. Production of Carbon Product (MMt) | Product Price ($2019/t) | U.S. Production of Coal-Based Carbon Product (MMt) | Potential U.S. Coal Production (MMt) |
|---|---|---|---|---|---|---|
| Carbon Product | 2019 | 2019 | 2050* | 2050 | 2050 | 2050* |
| Carbon Black | 1.5 | 1.5 | 2.3 | $939 | 1.8 | 13.1 |
| Engineered Plastic Composites | 1.5 | 2.4 | 108.1 | $2,706 | 86.5 | 51.9 |
| Activated Carbon | 0.7 | 2.3 | 11.3 | $2,035 | 9.0 | 30.1 |
| Anodes for Aluminum** | 3.4 | 1.1 | 1.5 | $3,674 | 1.2 | 2.8 |

## Workforce Impact




| | Projected Number of Manufacturing Jobs Created (2019) Based on Employment-to-Industry Output Ratio |
|---|---|
| Carbon Product | 2050* |
| Carbon Black | 3,400 |
| Engineered Plastic Composites | 294,200 |
| Activated Carbon | 37,700 |
| Anodes for Aluminum** | 9,300 |

# Process Analysis: Technoeconomic Analysis of NETL's Coal to Graphene (C2G) Process

NATIONAL ENERGY TECHNOLOGY LABORATORY

## Approach

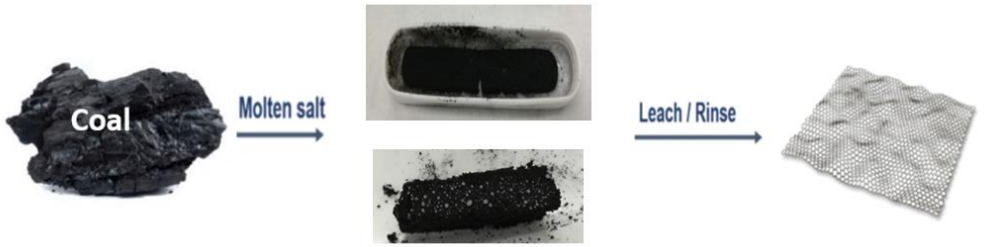
- Preliminary TEA conducted for NETL's C2G process
- Process Scale: = 4 tonnes/day coal, 2 tonnes/day carbon product

## Outcomes

- Quantified price reductions with comparison to current commercial products (graphite derived)
- TEA identified additional process improvements for NETL-RIC to investigate
- C2G TEA will be used to inform LCA in EY21

**NETL's C2G Process**

2020 R&D 100 WINNER




RAMACO CARBON

# Environmental Analysis of Coal Carbon Fiber & Use in Vehicle Light Weighting

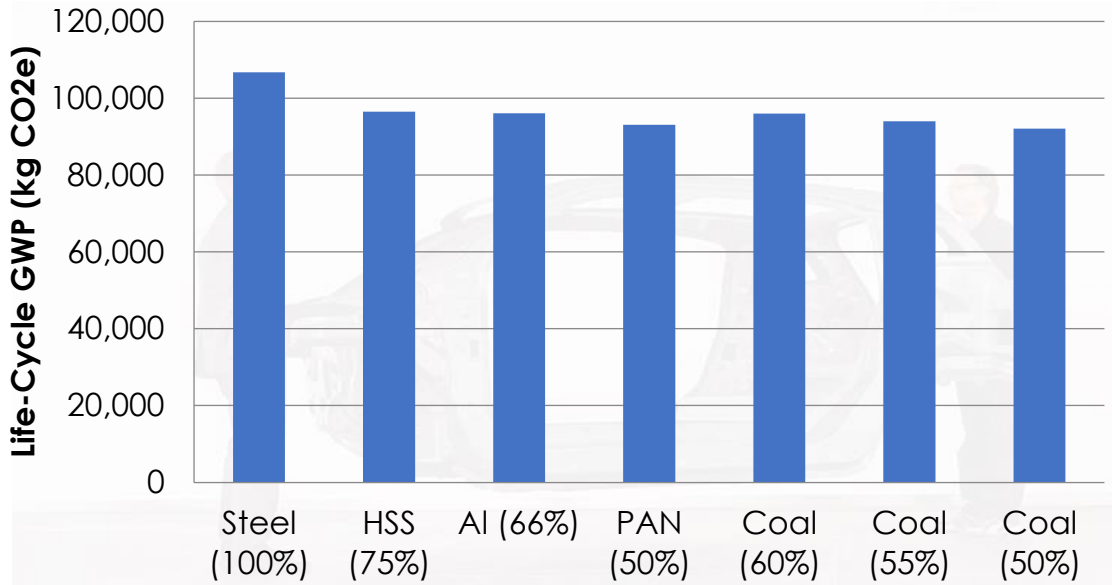
## Approach

- Screening study of coal-derived CFRP and vehicle light weighting initiated March 2020.
- Industrial stakeholders provided inventory data of coal CFRP manufacturing and automotive use.
- LCA compares life cycle environmental impacts of coal-derived CFRP, PAN CFRP, Steel, and Aluminum-bodied light vehicles.

## Outcome

- LCA study of coal-derived CFRP completed March 2021
- Initial draft of LCA journal manuscript is completed and currently under internal review process.

**Life-cycle Global Warming Potential for Vehicle Lightweighting Pathways**




HSS – High strength steel
Al – Aluminum
PAN – Polyacrylonitrile
Coal – Coal-derived CFRP

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- **American Coal Database**

# American Coal Database and Virtual Platform

## American Coal Databased (ACD)

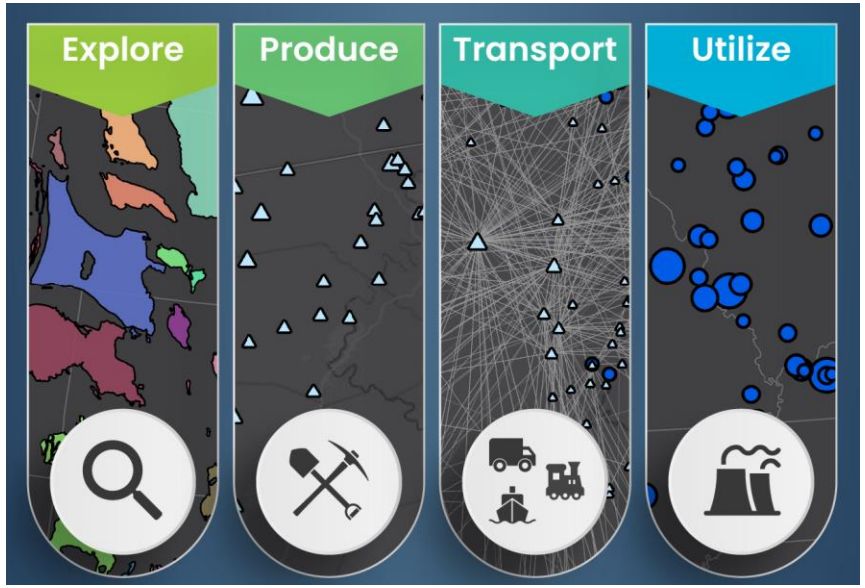
- Collection of existing coal databases from federal, state, university entities.
- Datasets updated to interface w/modern databases/computer codes
- Provides wide range of data on coal properties, geology/geochemistry, & supply chain/logistical issues

## Virtual platform (VP)

- Interactive web application that allows users to query the ACD to **collect, visualize, and analyze datasets**
- Enables **geospatial mapping** of data for geochemistry, geology, logistics/infrastructure, and coal seam properties

## ACD + VP will be publicly released via NETL's Energy Data Exchange (expected 2021)

https://edx.netl.doe.gov/




**Publication: Justman, D., Rose, K., Thomas, B. (Expected 2021). "A database and framework associated with US coal resources and supply chains." Technical publication under internal review.**

# Contents of the ACD

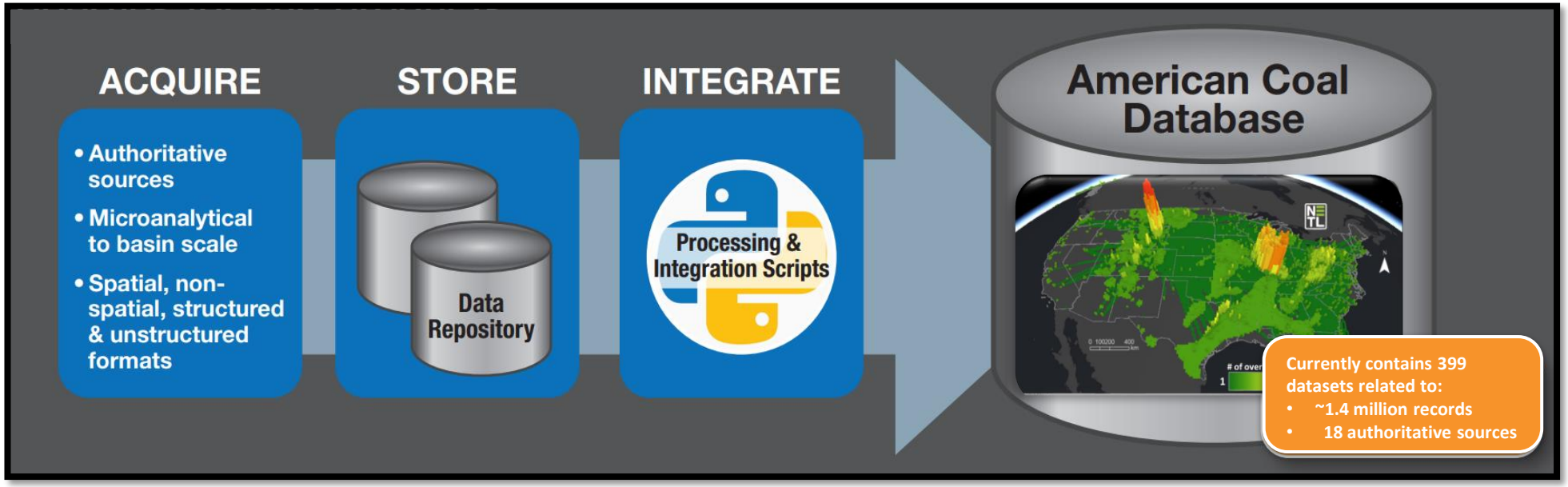
## Sources include

- USGS, EIA, state geologic surveys & agencies

## Contains

- 399 datasets
- ~1.4 M records

## What features and attributes does it contain?

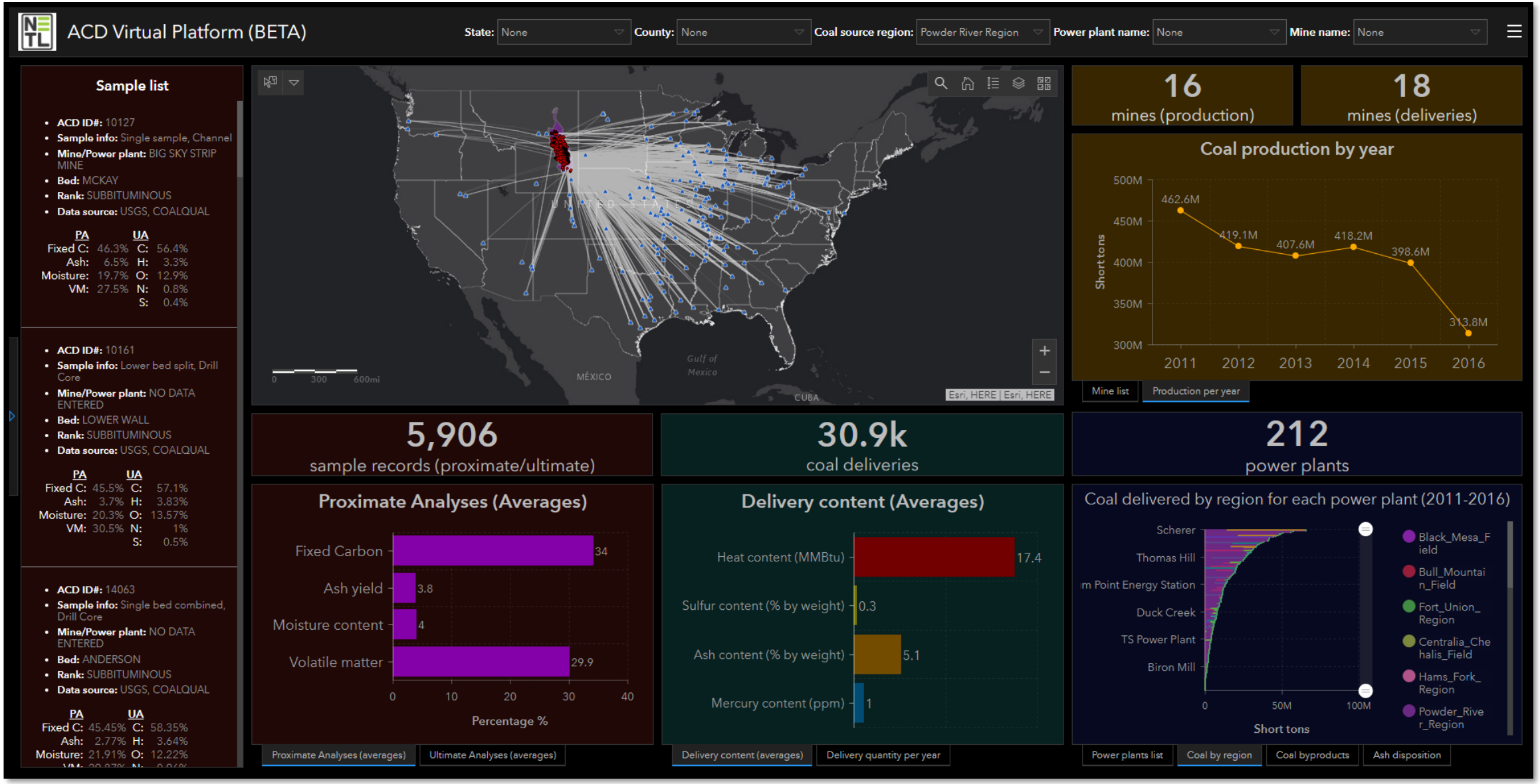



| Coal and ash samples | Geology | Mines | Coal deliveries | Power plants |
|---|---|---|---|---|
| •Proximate/ultimate analyses<br>•Oxides and trace elements<br>•Macerals<br>•Rank<br>•Others | •Coal bed geometries<br>•fields/basins/boundaries | •Production<br>•Deliveries from mine<br>•Coal region<br>•Location/operator information | •Quantity coal delivered<br>•Coal region<br>•Bulk ash/sulfur/ mercury content | •Consumption<br>•Quantity delivered from mine/region<br>•Byproduct quantity<br>•Ash disposition |



Justman, D., Rose, K., Thomas, B. (2021). A database and framework associated with US coal resources and supply chains. *Data in Brief*. In Review

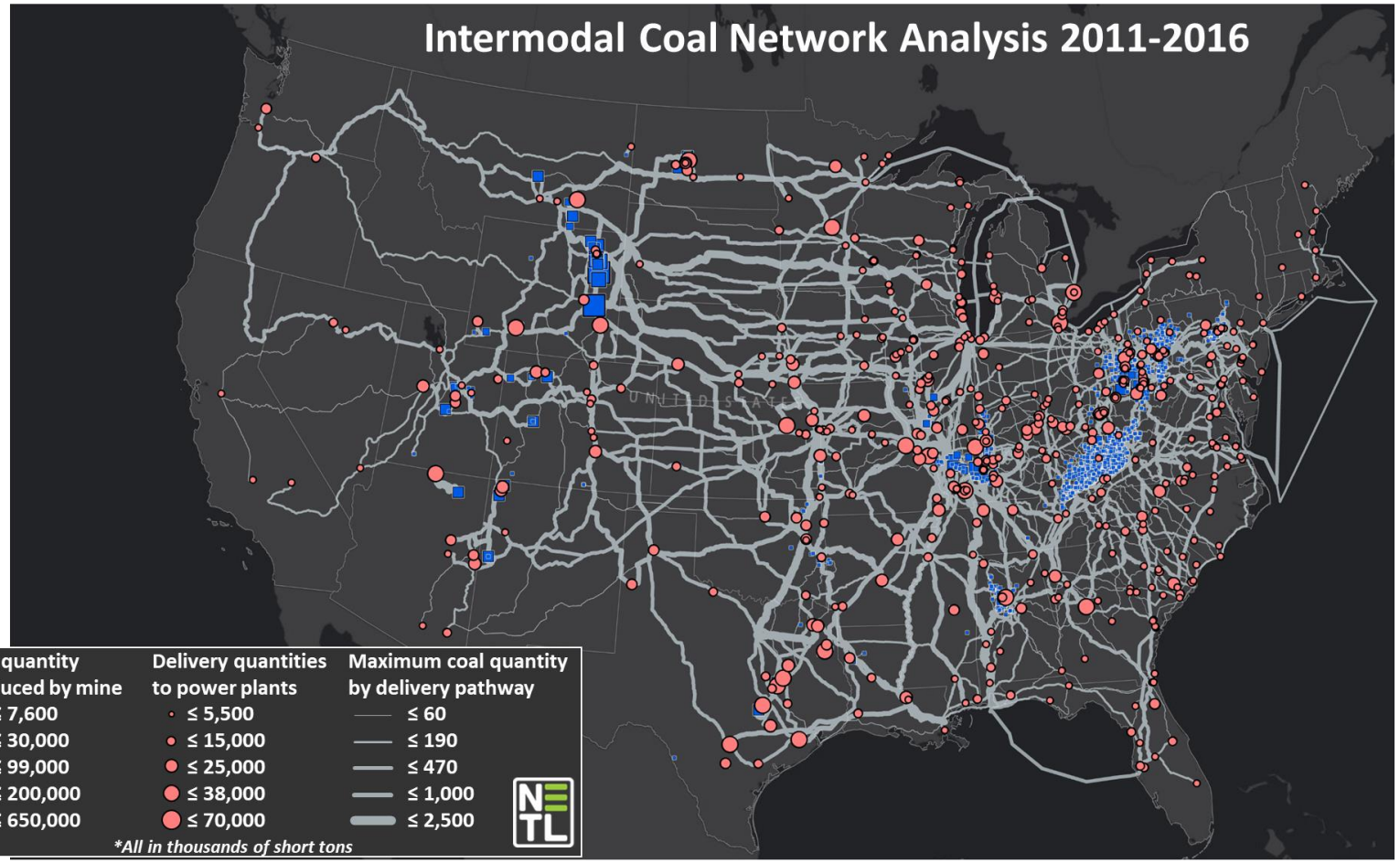
# ACD + virtual platform query: PRB Coal Production



# Future work

## Incorporate modeling efforts into virtual platform

- Coal beneficiation/products & carbon manufacturing products
- Improve transportation efficiency
- Identify supply chain hazards
- Optimizing supply chain networks



# Thank You!