NETL’s Intramural Research Program in Advanced Coal Processing

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Materials Discovery & Design

Market, Process, & Environmental Analysis

American Coal Database

COLLECT AND CATALOG DATA:

Coal production by mine (short tons)
- 10,000,000
- 15,000,000
- 20,000,000
- 25,000,000
- 30,000,000
- 35,000,000
- 40,000,000

Energy Data Exchange
Outline:

• Materials Discovery & Design

• Market, Process, & Environmental Analysis

• American Coal Database
Manufacturing Graphite from Domestic Coal and Coal/Biomass Blends

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
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

1-inch prototype
(~1000 Devices)

3-inch prototype
(~24,000 Devices)
Tunable Porous Carbon Materials From Powder River Basin Coal

PRB Coal

- Ultramicroporous carbons
  - S infiltration
    - Li-S batteries
- Microporous carbons
  - Gas Capture & Separations
  - Gas Capture/Storage/Separations
- Meso/micro porous carbon nanosheets
  - Metals loading
    - Supercapacitors
    - Single atom catalysts (HER, ORR, CO₂RR)

Today’s Focus
Tunable Pore Sizes, Highly Microporous

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

<table>
<thead>
<tr>
<th></th>
<th>BET SSA (m²/g)</th>
<th>QSDFT SSA (m²/g)</th>
<th>Ultramicropore volume ($\leq 0.7$ nm; cm³/g)*†</th>
<th>Micropore volume ($\leq 2.0$ nm; cm³/g)**†</th>
<th>Mesopore volume ($2.0 – 50.0$ nm; cm³/g)**†</th>
<th>Total pore volume (cm³/g)*</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ultramicroporous carbon</td>
<td>1480</td>
<td>2120</td>
<td>0.42 (55.3%)</td>
<td>0.62 (81.6%)</td>
<td>0.14 (18.4%)</td>
<td>0.76</td>
</tr>
<tr>
<td>Microporous carbon</td>
<td>2250</td>
<td>2440</td>
<td>0.41 (37.3%)</td>
<td>0.81 (73.6%)</td>
<td>0.29 (26.4%)</td>
<td>1.1</td>
</tr>
<tr>
<td>Mesoporous carbon</td>
<td>3500</td>
<td>2760</td>
<td>0.10 (5.6%)</td>
<td>0.85 (47.2%)</td>
<td>0.95 (52.8%)</td>
<td>1.8</td>
</tr>
</tbody>
</table>
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

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

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

Performance in other solvent systems

<table>
<thead>
<tr>
<th></th>
<th>Capacitance (F/g)</th>
<th>Rate capacity</th>
<th>Cycling stability</th>
<th>Energy Density (Wh/kg)</th>
<th>Power Density (W/kg)</th>
<th>Voltage (V)</th>
<th>Solvent</th>
</tr>
</thead>
<tbody>
<tr>
<td>NETL CNS</td>
<td>up to 200</td>
<td>55 %</td>
<td>&gt;90 %, 30,000 cycles</td>
<td>4.5-17.5</td>
<td>200-7,000</td>
<td>0-1.6</td>
<td>1 M Na₂SO₄</td>
</tr>
<tr>
<td>NETL CNS</td>
<td>up to 145</td>
<td>70 %</td>
<td>T.B.D.</td>
<td>20-42</td>
<td>700-14,000</td>
<td>0-3</td>
<td>1M TEABF₄ w/propylene carbonate</td>
</tr>
</tbody>
</table>
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# Market Analysis

## Products
- Carbon Fiber
- Graphene
- Carbon Fiber Cement
- Graphene Cement
- Roofing Tiles
- Carbon Composites
- Conductive Inks
- Carbon Foam
- Battery Anodes
- Carbon Black
- Engineered Composites
- Activated Carbon
- Al Anodes

## Market Impact

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

## Workforce Impact

<table>
<thead>
<tr>
<th>Carbon Product</th>
<th>Projected Number of Manufacturing Jobs Created (2019) Based on Employment-to-Industry Output Ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon Black</td>
<td>3,400</td>
</tr>
<tr>
<td>Engineered Plastic Composites</td>
<td>294,200</td>
</tr>
<tr>
<td>Activated Carbon</td>
<td>37,700</td>
</tr>
<tr>
<td>Anodes for Aluminum**</td>
<td>9,300</td>
</tr>
</tbody>
</table>
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
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.
Outline:

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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/

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
- Proximate/ultimate analyses
- Oxides and trace elements
- Macerals
- Rank
- Others

Geology
- Coal bed geometries
- Fields/basins/boundaries

Mines
- Production
- Deliveries from mine
- Coal region
- Location/operator information

Coal deliveries
- Quantity coal delivered
- Coal region
- Bulk ash/sulfur/mercury content

Power plants
- Consumption
- Quantity delivered from mine/region
- Byproduct quantity
- Ash disposition

Currently contains 399 datasets related to:
- ~1.4 million records
- 18 authoritative sources

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!