



# Fossil Energy Innovations

Oak Ridge National Laboratory (ORNL) has a rich history of scientific research supporting the nation's exploration, production, and use of abundant, domestic fossil energy. We focus on the R&D of materials and manufacturing for applications in extreme environments; modeling and simulation of subsurfaces; alternate uses of coal; and technologies for carbon capture, use, and storage.

## Materials and Manufacturing

- Materials-based solutions to advance modular fossil fuel power generation, with resulting improvements in fleet efficiency, flexibility, and resiliency
- Detailed characterization of novel materials to assist with ASME codification before first use in power plants
- Advanced manufacturing of new components for fossil energy production and use
- Development of computational tools for designing and predicting the performance of new alloys for advanced power generation technologies



*ORNL scientists developed a carbon nanospike catalyst that directly converts CO<sub>2</sub> and water into ethanol. The project won an R&D 100 award.*

## Carbon Capture, Use, and Storage

- Using additive manufacturing to design and develop an intensified packing device to enhance carbon capture at power plants
- Directly converting CO<sub>2</sub> to ethanol in a high-yield process using a nanotechnology-designed catalyst
- Using tracers to study the transport of CO<sub>2</sub> injected into the subsurface at the Cranfield site in Natchez, Mississippi—a unique, real-world test of CO<sub>2</sub> storage
- Developing models to predict the long-term security of CO<sub>2</sub> storage sites
- Demonstrating a new energy-efficient, direct-air-capture approach to CO<sub>2</sub> that recycles sorbent materials



**INNOVATING**  
materials and sensors for power plants



**ENGINEERING**  
sorbents, solvents, and membranes for CO<sub>2</sub> solutions



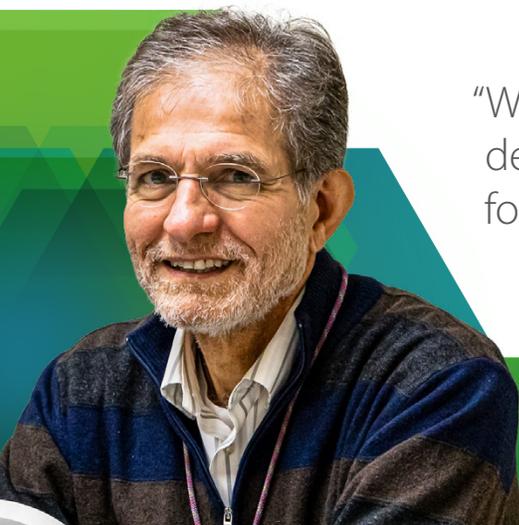
**DEVISING**  
advanced algorithms to image subsurfaces



**MODELING** concepts with supercomputing to speed research



**CONVERTING**  
coal into high-value products like carbon fiber



“We designed and demonstrated an additively manufactured device that significantly enhances carbon dioxide capture for fossil fuel plants and other industrial emissions.”

**Costas Tsouris, Distinguished R&D Staff**

# Comprehensive Capabilities

**High-performance computing (HPC)**—The nation's fastest supercomputer for open science, modeling power generation and the subsurface environment

**Neutron science**—Two of the most powerful neutron science facilities in the world, providing a nondestructive, atom-level view of materials and processes

**Center for Nanophase Materials Sciences**—Providing access to expertise and equipment for nanomaterials synthesis, nanofabrication, imaging, microscopy, and modeling for materials characterization

**Carbon Fiber Technology Facility**—The US Department of Energy's only designated user facility for carbon fiber innovation, developing high-potential, low-cost precursors, including coal

**Manufacturing Demonstration Facility**—Developing new manufacturing technologies to reduce the cost of materials for carbon capture and storage, modular power generation, coal gasification, and coal-to-products innovations

**Battery Manufacturing Facility**—Analyzing every aspect of battery production, from raw materials and electrode preparation to finished product and performance testing

**Extreme environment evaluation and testing**—ORNL houses a large fleet of unique high-temperature corrosion, fatigue, and creep-test equipment

**Chemical and molecular science, engineering**—Applying fundamental research to separations, sequestration, and power generation processes

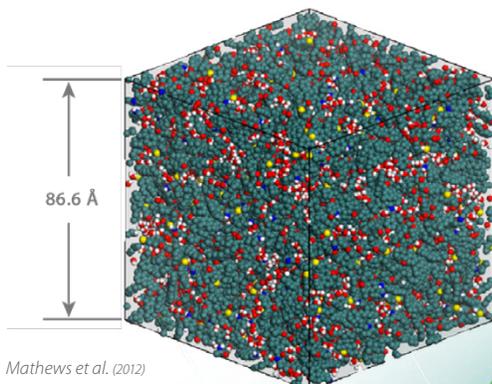
## Coal-to-Products

ORNL is using coal-derived feedstocks for:

- Manufacturing carbon fibers with tunable physical and mechanical properties at semiproduction scale at the Carbon Fiber Technology Facility
- Manufacturing low-cost anodes with high capacity and durability for lithium-ion and sodium-ion batteries at the Battery Manufacturing Facility

ORNL is also developing a virtual laboratory to enable the development of cost-effective, energy-efficient, and environmentally sustainable processing technologies to obtain coal-derived feedstocks for manufacturing high-value products. Key components of the virtual laboratory include:

- A methodology for characterizing coals, not based on their calorific value or their concentration of carbon, ash, and moisture, but on their molecular structure
- Scalable quantum chemical and machine-learning approaches for accurate prediction of coal reactivity based on its structure



Mathews et al. (2012)

## HPC4Materials

*The HPC4Materials program provides industry partners access to HPC systems and expertise at the national laboratories. ORNL is collaborating with industrial partners to accelerate the discovery, design, and development of materials for applied energy technologies, including power generation and the production of hydrogen from fossil fuels without CO<sub>2</sub> emissions.*



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