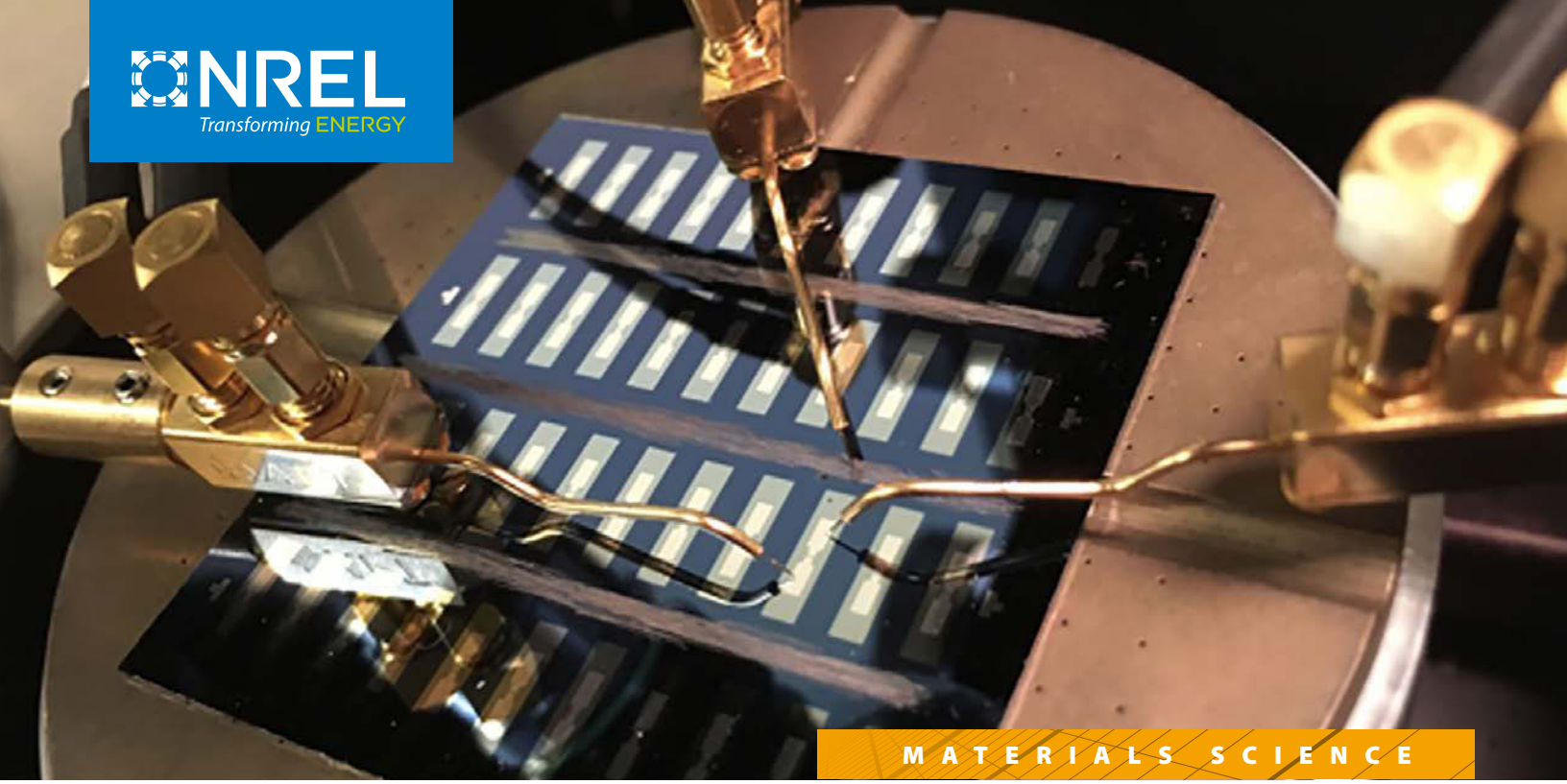



High-throughput testing of thin-film transistors. *Photo by Sage Bauer, NREL.*

# Materials Discovery

**Advanced energy technologies are enabled by the constituent materials found in functional devices. Scientists at the National Renewable Energy Laboratory (NREL) are leaders in discovering the new materials that provide the foundation for future innovations.**

## Use-Inspired Fundamental Research

Our research aims to discover new materials for energy applications by using high-throughput, combinatorial experimental research methods. Materials discovery team follows an ethos of "material design," working with computational colleagues to predict the most functional materials from their underlying physical and chemical properties—before ever stepping into the lab. We also work closely with application experts, both internal and external, to rapidly assess and develop application-specific optimized materials.

Some examples include:

- Photoabsorbers
- Transparent conductors
- Battery materials
- Quantum materials
- Piezoelectrics and Ferroelectrics
- Catalytic materials
- Memory materials
- Materials for electronics.

## High-Throughput Experiments

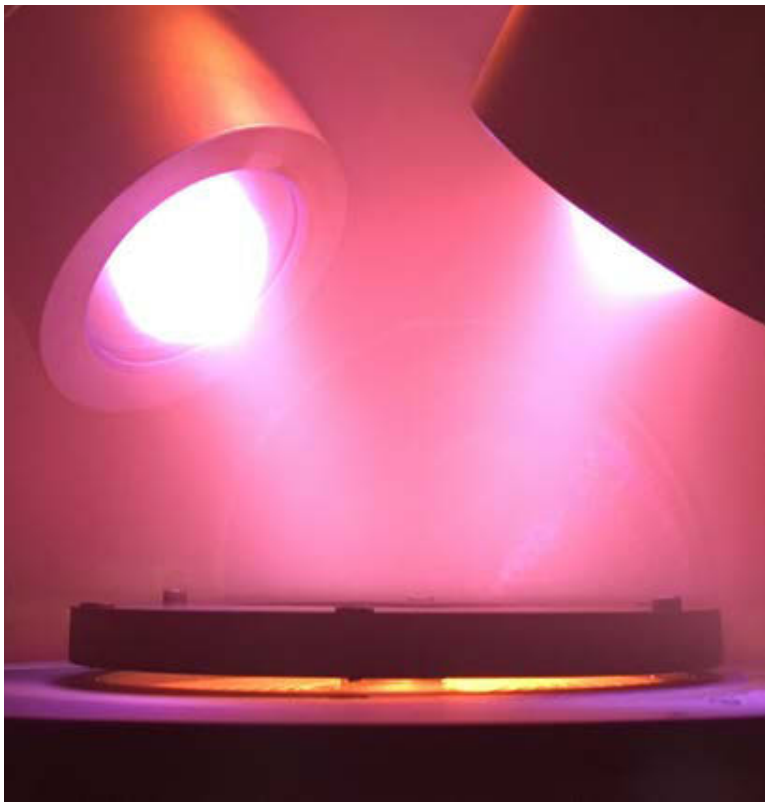
Material screening using combinatorial research strategies allows for dozens of materials to be evaluated in parallel. This accelerates the pipeline for discovery, development, optimization, and adoption of new energy materials. NREL employs a suite of custom experimental tools that help enable this research:

- Multi-source sputtering (up to four sources)
- Radio frequency (RF), direct current (DC), and RF+DC sputtering

- Pulsed laser deposition (up to six sources)
- Complex programmable shuttered operation
- Composition mapping (X-ray fluorescence [XRF], Rutherford backscattering spectrometry [RBS])
- Structure mapping (X-ray diffraction [XRD], X-ray reflectivity [XRR], microscopy)
- Thickness mapping (XRR, XRF, profilometry)
- XRD, XRR with in situ annealing (T < 1,100°C)
- Optical properties mapping (UV-Vis, spectroscopic ellipsometry, Raman, X-ray photoelectron spectroscopy [XPS])
- Electronic properties mapping (4-proton photoemission [4PP], Hall, Seebeck, Kelvin probe)
- Data management software
- Publicly accessible materials database.

## The Periodic Table is Our Playground

The materials discovery team works with a range of materials chemistries including carbides, silicides, nitrides, phosphides, antimonides, oxides, chalcogenides, halides, and intermetallics. We also work with materials in powder, thin-film, 2D, and single-crystal forms. This breadth of experience means we are ready to experimentally explore any newly predicted material.



**Thin-film growth in reactive plasmas.** *Photo by Andriy Zakutayev, NREL.*

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## Learn More

**NREL Materials Discovery**
*www.nrel.gov/materials-science/materials-discovery.html*

**COMBIgor: Data-Analysis Package for Combinatorial Materials Science**
*https://github.com/NREL/CombIgor*

**HTEM DB (High Throughput Experimental Materials Database)**
*https://htem.nrel.gov*


NREL Transforming ENERGY

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