# LLNL Capabilities in Materials Modeling, Characterization, and Synthesis for Module **Reliability Improvement and Cost Reduction**

#### **Overview**

Unique capabilities in computational and experimental materials design, characterization, and synthesis enable accelerated insertion of new, high-performance materials throughout the solar module to improve reliability, extend lifetime, and reduce cost.

# Materials Design and Discovery using High-Performance Computing



- Spanning the atomic-scale, mesoscale, and macro-scales, from first-principles to continuum
- Coupled-scale models allows accurate prediction of device and system response with few parameters





Fermi level pinning from defects reduce conductivity of TCO Hydrogen in SnO<sub>2</sub> VBM VBM Conduction Conduction band Valence band Valence ban

**Transparent contact degradation** 

HPC resources, access, and support

These computational tools, combined with world-leading HPC, enable the design and search of improved materials for module components for longer lifetimes, higher reliability, and/or reduced cost.

**Kinetics of phase transformations** and defect evolution

**Interfaces and defects** 

Polymer degradation



## Infrared Spectroscopy of Water **Ingress in Solar Modules**

• Non-destructive study and qualification of long-term reliability of (flexible) modules related to water ingress into and through polymer encapsulants



Infrared signatures of water ingress in multiple transparency windows

## **Dynamic Transmission Electron Microscopy (DTEM)**

• Unique instrument invented at LLNL for direct imaging of materials transformations at the sub-ns and sub-nm scales • Enables the study of reactivity, stability, and strength of materials, especially at interfaces, with unprecedented detail



15 nm time resolved images



#### **Additive Manufacturing of Hierarchical Metamaterials**

• Fabrication of metamaterials with enhanced properties and

0.5 µm

Hierarchically structured broadband absorptive coating

0.25 µm



Large-area 3D architected metamaterials with features spanning 7 orders of magnitude

Lawrence Livermore

**National Laboratory** 

800

500 600 700 Wavelength nm

700

400

#### **TECHNICAL REPRESENTATIVES**

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0.5 µm

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