

Long-range Challenges

NREL's Materials and Computational Science Center performs world-class research and provides the knowledge base to meet long-range fundamental challenges in renewable energy production and storage. This includes:

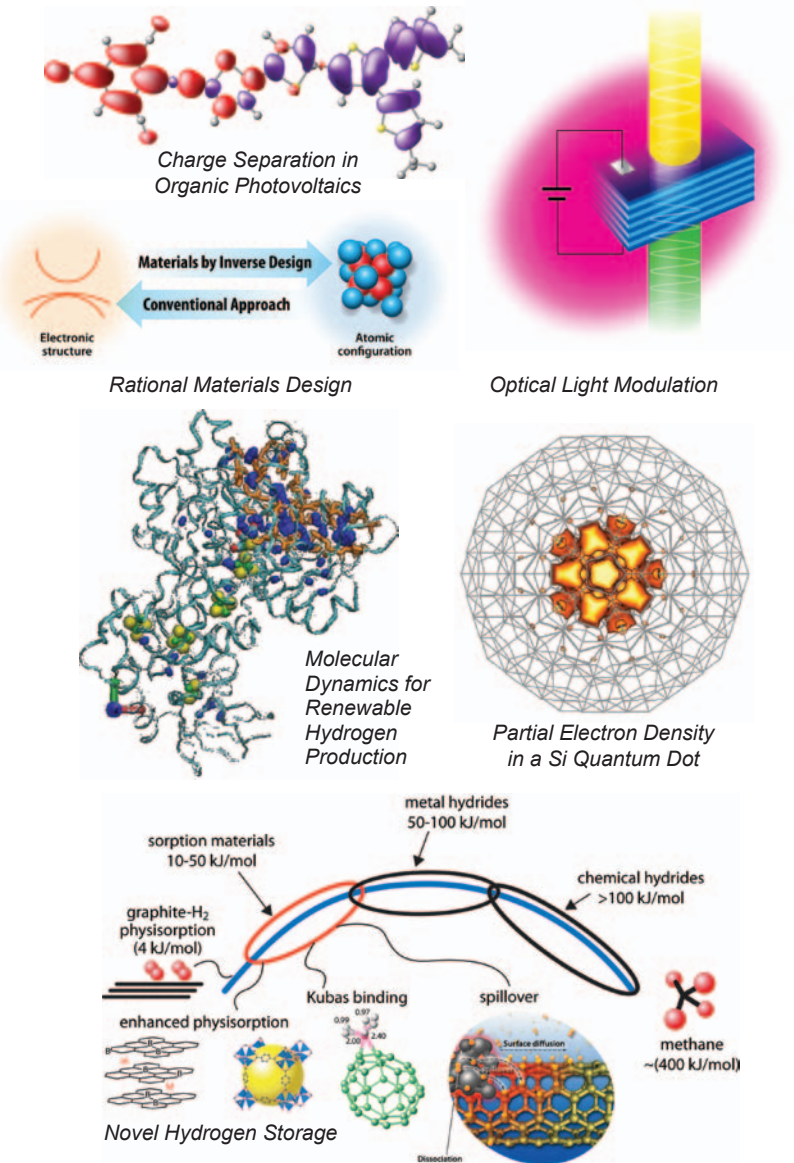
- Theoretical calculations to select and optimize the materials used in modern optoelectronic devices
- High performance computing, numerical simulation, and scientific data management
- Synthesis and characterization of advanced energy generation and storage materials.

In addition, the Center:

- Models and predicts the properties of complex materials and guides experimental research
- Enables simulation based on fundamental physical principles and mathematical models
- Collects, analyzes, and investigates of results from complex experimental, high through-put, and simulation-based methods
- Synthesizes and characterize nanostructured materials for batteries, hydrogen storage, electrochromic windows, and high temperature superconductor films
- Utilizes ultrafast optical spectroscopies and magnetotransport measurements to investigate the properties of materials used for renewable energy technologies.

Research Capabilities

- First-principles calculations and large-scale material simulations
- High performance computing and stereo 3D data visualization
- Scientific data management and analytics
- Inductively coupled plasma (ICP) analysis; high energy and reactive species synthesis
- Precision analysis of hydrogen, methane, and carbon dioxide adsorption thermodynamics
- X-ray diffraction; Nuclear Magnetic Resonance
- National test facility for commercial dynamic windows
- Ultrafast, high-magnetic field, and submicron spatial resolution optical spectroscopy



Research Focus Areas

- Materials theory and knowledge-based materials design
- High performance computing and numerical simulation
- Materials for ultracapacitors and smart windows
- Scientific data management, analytics, and visualization
- Materials for efficient renewable energy conversion and storage (hydrogen, electrical, heat)
- Spectroscopy of solid state materials

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