NREL

ADVANCED COMPUTING
ANNUAL REPORT
2024

A Note From the Director

In Fiscal Year (FY) 2024, the National Renewable Energy Laboratory (NREL) took a major leap forward with the completed full buildout of Kestrel, the U.S. Department of Energy's Office of Energy Efficiency and Renewable Energy's newest high-performance computing (HPC) system. Kestrel is already supporting science across the portfolio, bringing roughly 44 petaflops of computing power, which is more than five times the capacity of our previous supercomputer, Eagle. By delivering greater GPU capacity, Kestrel enables faster progress in artificial intelligence (AI) and opens new avenues in energy research—from defining long-term planning scenarios to accommodate a growing power system to material discovery to improving energy efficiency in photovoltaics (PV). Across the portfolio, research is being accelerated by Kestrel's impressive power.

During FY 2024, 427 projects and more than 700 researchers used NREL's HPC, supporting the Office of Energy Efficiency and Renewable Energy across 13 funding areas. Through these collaborations, researchers produced more than 450 technical outputs, including 195 articles in peer-reviewed publications, pushing the boundaries of science and engineering.
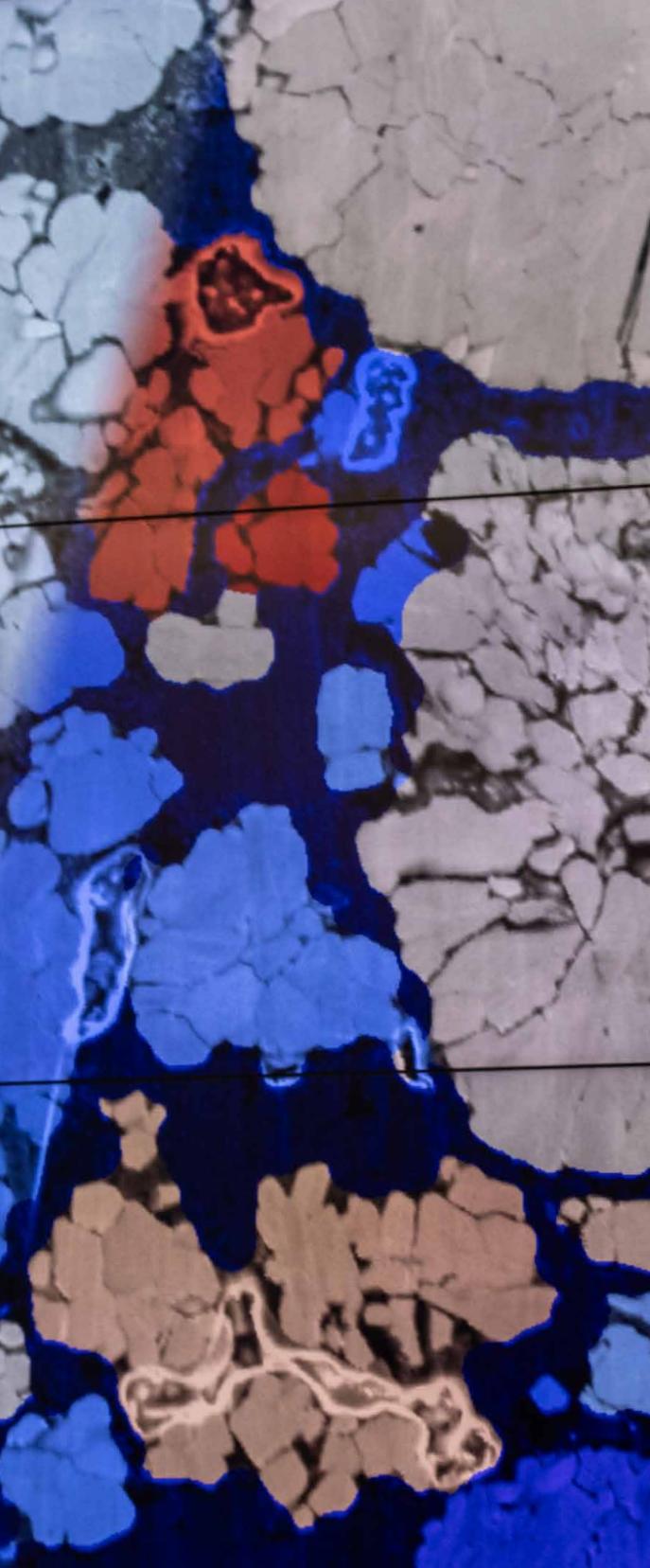
This year's report features new sections spotlighting the expanding roles of AI and accelerated computing. We also introduce an early career section to celebrate the accomplishments of our up-and-coming researchers, whose pioneering work is shaping the future of energy. We hope you enjoy the new insights and discoveries highlighted in these pages.

Ray Grout,
Director, Computational Science Center

Kris Munch,
Laboratory Program Manager, Advanced Computing

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CAPABILITIES AND PROJECTS

AT A GLANCE

Patent on Perovskite Materials for Efficient Hydrogen Production

Kestrel supported development of a new patent describing a novel class of quinary metal oxide perovskite materials optimized for efficient hydrogen production using sunlight and water in a two-step thermochemical cycle. This innovation has the potential to significantly advance hydrogen technology, offering a scalable pathway for energy generation.

Early Career Award Winner Models Extreme Events in Complex Systems

Early career funding supports enrichment of computer models of extreme events.
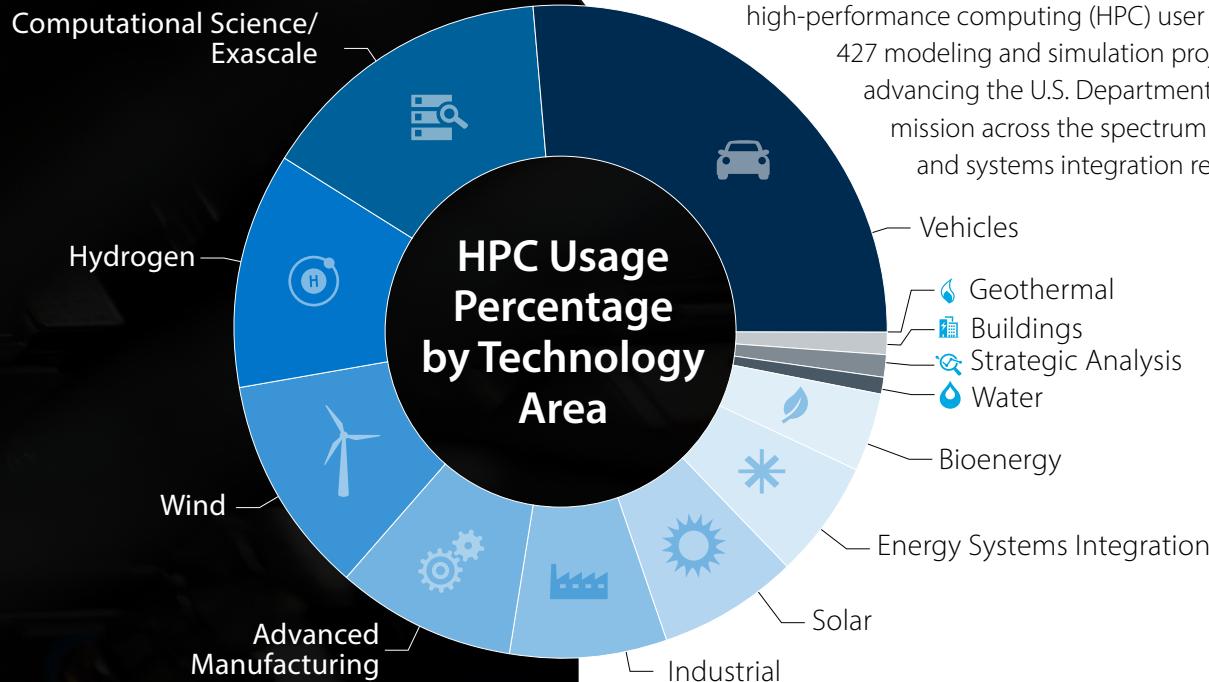
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706 Total users

88% HPC availability

90% HPC utilization

427 Modeling and simulation projects

MODELING AND SIMULATION PROJECTS

The National Renewable Energy Laboratory's (NREL's) high-performance computing (HPC) user facilities supported 427 modeling and simulation projects in FY 2024, advancing the U.S. Department of Energy (DOE) mission across the spectrum of energy technologies and systems integration research.

HPC Usage Percentage by Technology Area

- Computational Science/Exascale
- Hydrogen
- Wind
- Advanced Manufacturing
- Industrial
- Solar
- Energy Systems Integration
- Bioenergy
- Water
- Strategic Analysis
- Buildings
- Geothermal
- Vehicles

Kestrel Supercomputer Energizes Energy Research

After more than 2 years of hard work, the Kestrel supercomputer buildout is complete, providing 44 peak petaflops of computing power focused on energy technologies and systems integration research. Built by Hewlett Packard Enterprise, the HPC system boasts more than five times the computing power of the DOE Office of Energy Efficiency and Renewable Energy's (EERE's) previous supercomputer, Eagle.

The work to install Kestrel in NREL's Energy Systems Integration Facility HPC data center kicked off with the arrival of the first phase of equipment—including CPUs and a 95-petabyte parallel file storage system—in March 2023. In November 2023, the remainder of the CPUs landed Kestrel at #67 on the 62nd edition of the TOP500, an industry-standard list of the 500 most powerful computers in the world, showcasing 14.3 petaflops of performance from Kestrel's CPU capability alone.

With the summer 2024 completion of the installation, Kestrel now has 132 GPU nodes—each hosting four NVIDIA H100 GPUs—added to the 2,314 existing CPU nodes. The GPUs are already in use by more than 100 projects, elevating the work at EERE to new heights by enabling emerging artificial intelligence (AI) and machine learning (ML) workflows.

Now that Kestrel is fully complete, GPUs and all, researchers are plugging in and using Kestrel's power to accelerate energy research, driving advancements in energy technologies and systems integration.

Situated Visualization of Photovoltaic Module Performance

NREL has expanded the capabilities of the Insight Center by adding **situated visualization**, which overlays digital information onto physical objects or environments, enabling users to explore data in a way that is spatially mapped onto the physical world. For example, users can adjust the orientation of a physical solar photovoltaic (PV) module in the lab and immediately see real-time performance changes visualized on the PV module itself. This interactive approach bridges the gap between abstract data and tangible systems, making it easier for analysts to grasp the relationship between environmental factors and system performance.

This capability is especially useful for analyzing energy systems where real-world variables, such as sunlight angle or shading, can significantly impact performance. And, by incorporating augmented reality and real-time feedback alongside the new situated visualization tools, the Insight Center now offers more immersive and hands-on experiences for scientific exploration and training.
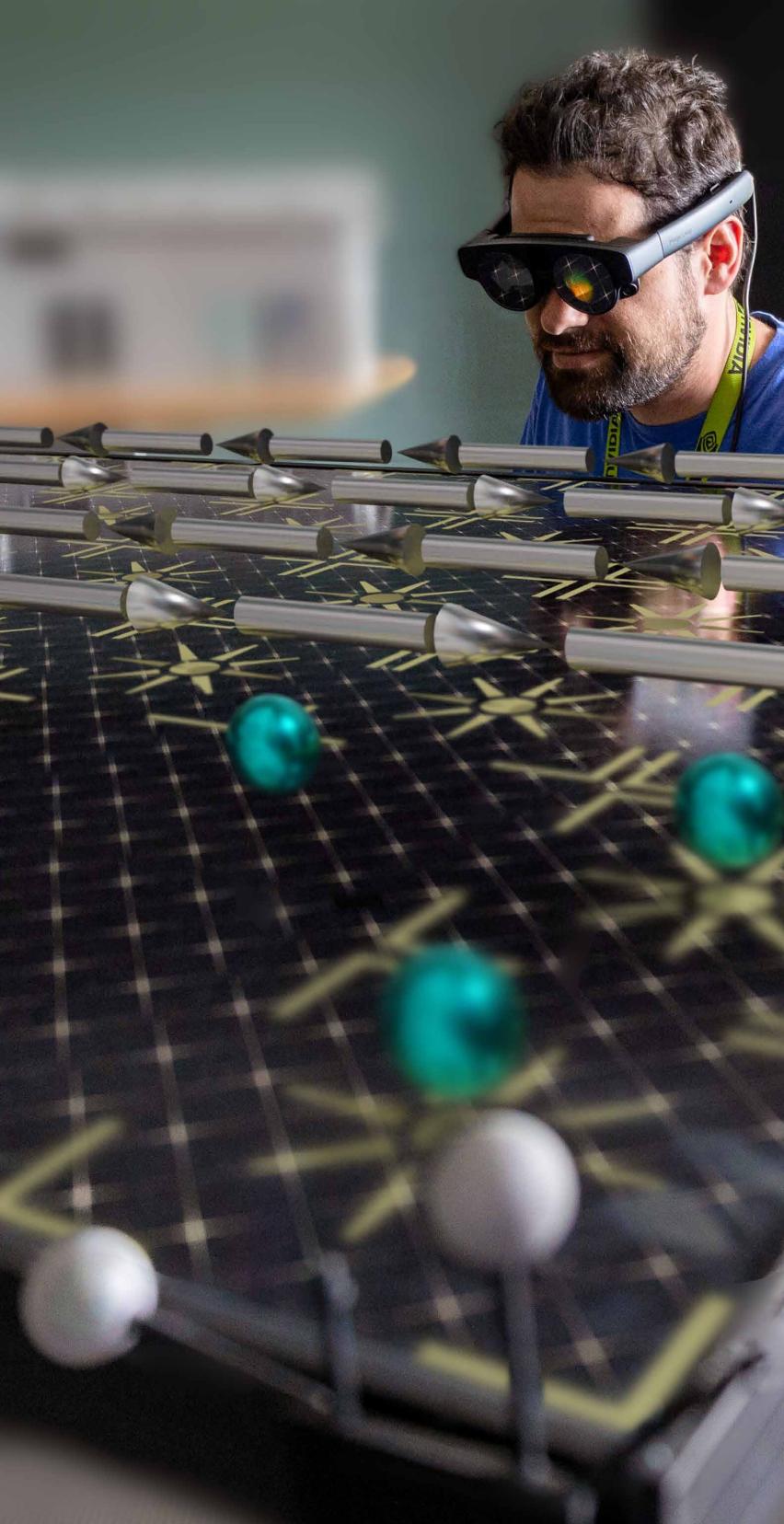
Tool Highlights Hydrogen Cost-Reduction Strategies for Large-Scale Industrial Use

To provide high-fidelity visualizations of hydrogen costs across the country, NREL researchers needed a platform with the capability to provide data for more than 50,000 U.S. hybrid energy plant locations. The Hybrid Environment Resources and Operations (HERO) tool helped the team visualize the performance of a hybrid wind-solar plant with levelized cost of hydrogen to make suggestions for cost reduction strategies and specifically identify locations with promising key attributes.

HERO supports mission-driven research projects by providing a set of common web services and reusable software components to support advanced computational workflows across cloud and HPC. HERO maintains metadata for project workflows and stores data in both cloud data repositories as well as local on-premise data systems, enabling access to data via common APIs. The architecture of HERO enables engineers and researchers to develop and deploy their own HERO applications and leverage common HERO services, thus lowering the barriers to computational resources by making it easier and faster to build and use workflows. HERO is transforming energy research by revolutionizing scientific workflows, discovery, and collaboration.

ARTIFICIAL INTELLIGENCE AND ACCELERATED COMPUTING
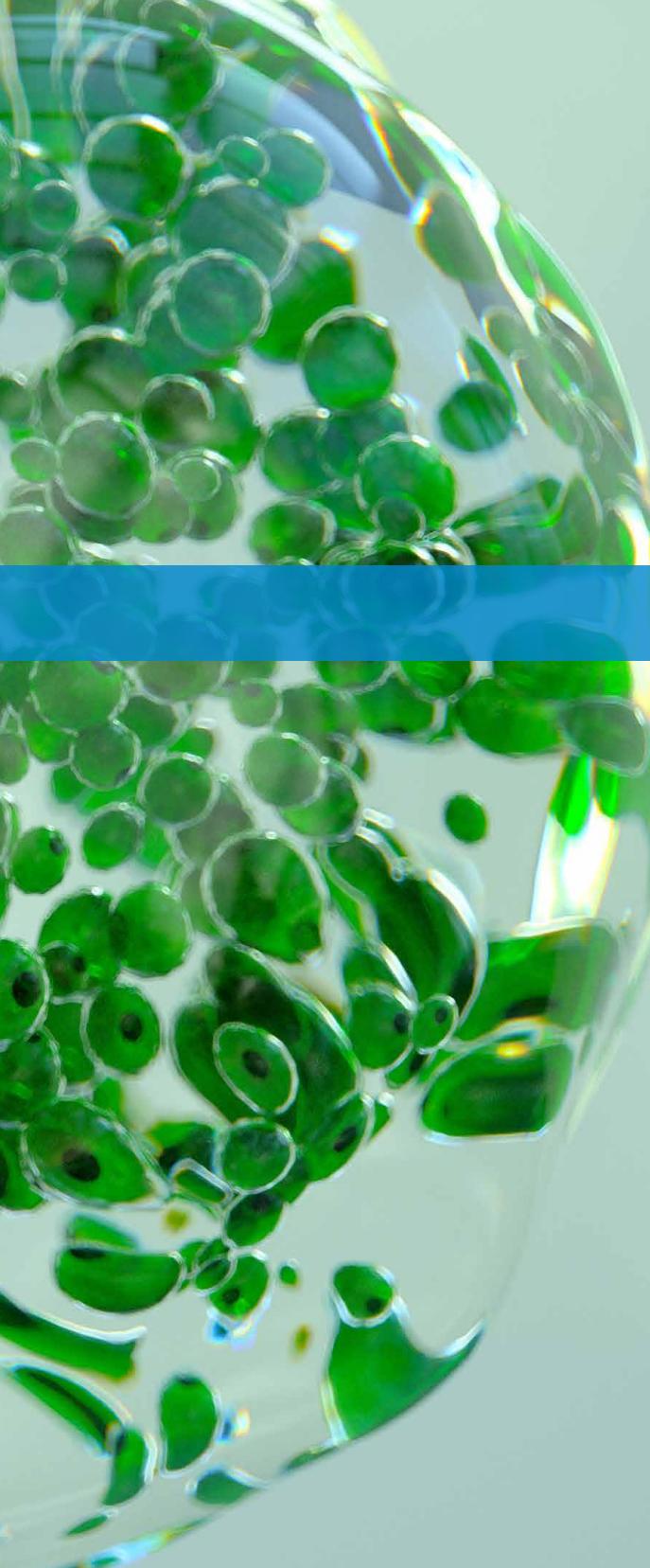
Reducing Costs of Bioderived Products and Materials

The Biochemical Process Modeling and Simulation project, supported by the DOE Bioenergy Technologies Office, deploys modeling and simulation tools at length scales ranging from atomic to reactor, with an overarching objective to streamline experimental and engineering efforts to reduce the cost of bioderived products and materials by addressing process bottlenecks.

A major challenge in biochemical platforms is engineering microbes and their enzymes, which convert biomass to valuable products, to withstand harsh conditions such as high temperature, acidic pH levels, and high concentrations of products such as ethanol. NREL researchers are leveraging the GPUs on Kestrel to develop ML techniques to predict how enzymes can be modified to increase their stability. In addition, the team is developing GPU-accelerated high-throughput molecular dynamics simulations to model the effects of harsh conditions for a large variety of proteins, which will also feed more data to train the ML models. In tandem, these approaches have the potential to greatly improve the effectiveness of enzyme engineering campaigns and ultimately increase the efficiency of producing new fuels and chemicals.

Next-Generation AI for Complex Energy Systems

Scientific ML is becoming increasingly useful to replace or supplement models for computational physics problems; however, many ML approaches require a vast array of training data and can struggle with generalization and interpretability. As part of an NREL Laboratory Directed Research and Development project called AI Architectures for Reduced Order Modeling (AIROM), NREL scientists used differentiable simulators and next-generation AI architectures to learn surrogate models for complex simulations. In particular, the team applied Fourier Neural Operator architectures to learn surrogates of large eddy simulations, setting the stage to enable AI versions of large-scale turbulence models to be used for industrial applications like wind farm design.

Separately, the team used differentiable simulators in an AI training loop to teach a multi-scale surrogate to better connect particle-scale and reactor-scale modeling of biomass pyrolysis. By using AI to connect these model scales, they drastically improved the reliability of pyrolysis yield simulations to better match experimental results with an extremely small number of training simulations.

Modeling Extreme Events in Complex Systems

Motivated by the drastic impacts of extreme environmental events on human and natural systems, NREL computational scientist Julie Bessac, Ph.D., is pursuing work on developing novel statistical and ML models to advance the understanding and modeling of extreme events arising in complex systems. With her recent award funding under the DOE Office of Science's 2023 Early Career Research Program, Bessac is working to correct or enrich computer models for environmental conditions that derive from classic physics-based models. Classic models omit details and may lead to misevaluated risks for systems and living populations susceptible to extreme environmental stressors. This knowledge gap around extremes results in inadequate response and increased exposure or cost. Using Kestrel, Bessac's team demonstrated that a statistical treatment of classical super-resolution neural networks reveals fine-scale features of wind fields. As some models may understate the potential for environmental conditions, especially extreme events, updating models will enable leaders and people to prepare for current and future climate conditions.
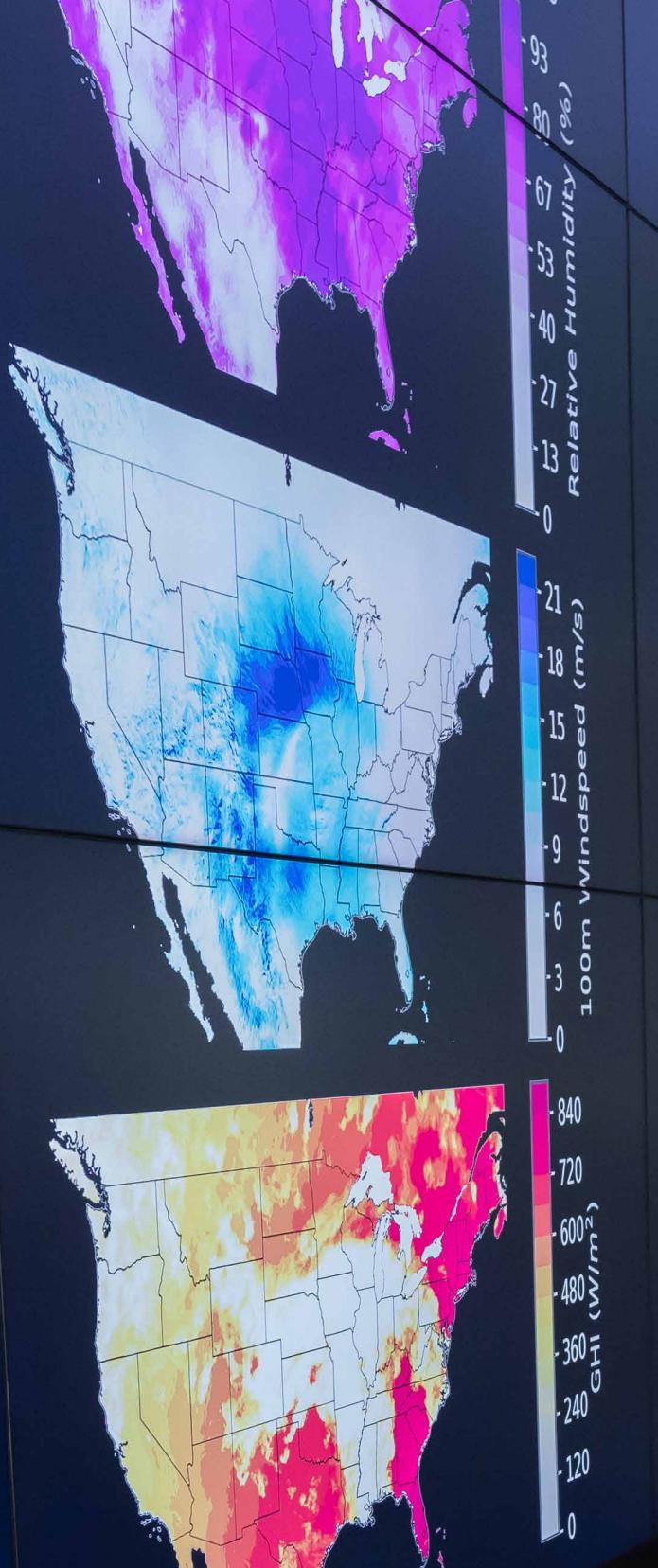
Designing Advanced Catalysts With Boost From AI

With funding from the DOE Office of Science's Beyond-DFT Electrochemistry with Accelerated and Solvated Techniques (BEAST) project, NREL researchers and collaborators from Rensselaer Polytechnic Institute, Lawrence Berkeley National Laboratory, the University of Colorado Boulder, and the University of South Carolina are designing better catalysts for water electrolysis, fuel cells, and carbon dioxide reduction. The BEAST team, which is focused on high-fidelity simulation of electrocatalytic systems beyond standard density-functional theory (DFT) approaches, developed and paired new, GPU-accelerated algorithms with AI to achieve an unprecedented description of electronic structure in both speed and scale. Leveraging Kestrel, they performed high-fidelity, beyond-DFT random phase approximation calculations for a range of electrocatalysts and adsorbates, including previously unachievable calculations. Kestrel enabled the BEAST team to run both standard catalytic model sizes on 8 GPU nodes, up to complex models requiring 64 GPU nodes. The BEAST team will utilize this scaling of the random phase approximation method on Kestrel GPU nodes to generate corrections to their DFT calculations in BEAST Database (beastdb.nrel.gov), the recently published database of electrocatalytic calculations.

In parallel, the team developed an AI approach that combines graph neural networks and an efficient description of electronic states to predict high-fidelity electronic structure of electrocatalysts at the cost of lower-fidelity DFT calculations. This graph neural network approach greatly improves predictions for heterogeneous catalytic systems due to its ability to capture local active site structure. The ability to simulate complex models of catalytic systems and build large databases of catalysts with high fidelity will advance understanding of the factors that determine electrocatalytic performance.
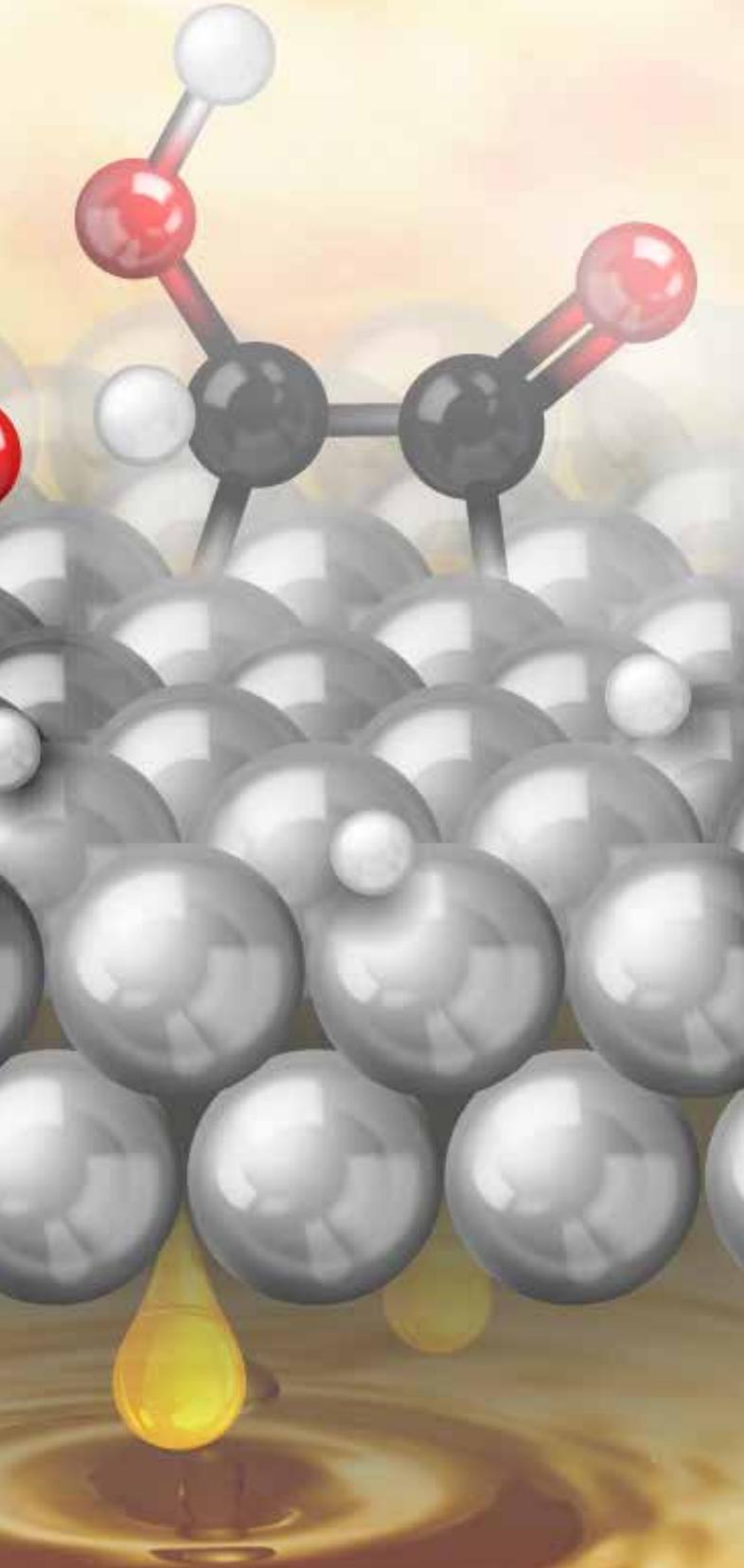
Multiscale, Multiphysics Simulation Tool Optimizes Battery and Device Performance

All-solid-state batteries are one of the most promising energy storage technologies with improved safety and energy density, though stability issues have hindered deployment in a wide range of applications. Understanding chemo-mechanical degradation at interfaces that impede performance and promote failure, as well as how these can be controlled at multiple length scales, is key to realizing targeted design and optimization of all-solid-state battery architecture. Funded by the DOE Vehicle Technologies Office and led by Lawrence Livermore National Laboratory, the team applied multiscale, multiphysics simulation tools to probe the mechanisms of failure at interfaces, including changes in chemistry and mechanical properties. Aided by Kestrel's GPU acceleration ability, the team developed machine-learned surrogate models to enable high-fidelity, large-scale molecular dynamics simulations of thousands of atoms with quantum-level accuracy, which were used to directly simulate interfacial evolution and degradation. They also incorporated these results within larger-scale models of composite materials to probe how stresses evolve during simulated battery cycling. Overall, these multiscale modeling tools are a first step toward enabling rational design of interfaces and optimization of device performance of all-solid-state batteries.

INTEGRATED ENERGY SYSTEMS
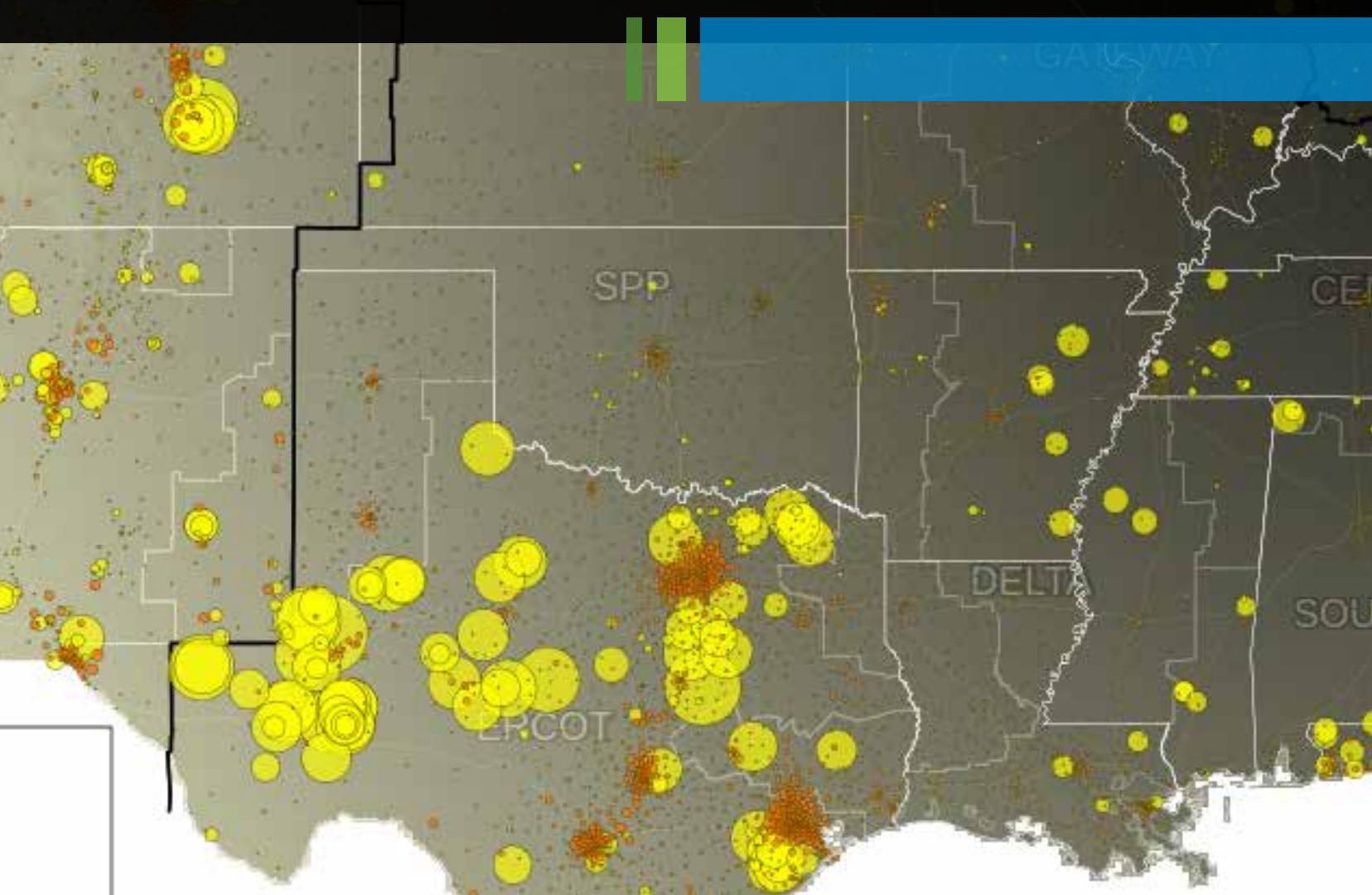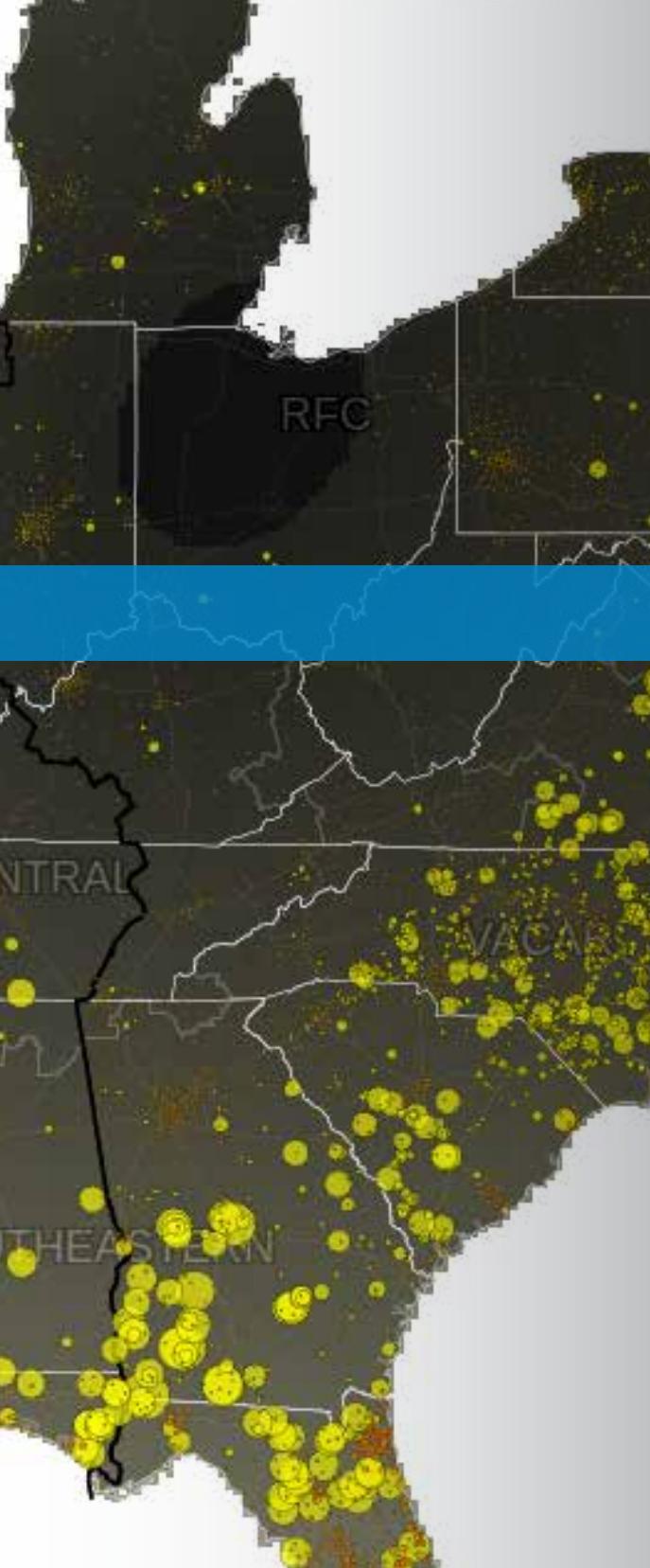
Total Solar Eclipse

On April 8, 2024, NREL researchers transformed the Insight Center into an eclipse command center to monitor and analyze the real-time impacts of the total solar eclipse on the nation's electrical grid. They displayed real-time data feeds from multiple independent system operators, providing a dynamic view of solar generation as it rapidly decreased and recovered across the United States. Visualizations showcased high-resolution, detailed animations that tracked rooftop and utility-scale solar installations in regions such as California, Texas, and New York.

Visualization experts facilitated precalculated impact assessments, developed prior to the eclipse, to anticipate how different regions would respond. These high-resolution visualizations—based on detailed models integrating weather, solar, and grid data—allowed researchers to explore the eclipse's potential effects on interconnections, independent system operators, and balancing authorities across various spatial scales—from individual plants to larger grid sectors. Visualizing this data with such precision proved invaluable for assessing the solar eclipse's impact, as it provided a clear visual representation of the effects on the grid. By blending real-time monitoring with high-fidelity pre-event modeling, the eclipse command center allowed researchers to fully understand the complex interactions between solar generation and grid operations, ensuring that future visualization tools offer the granularity needed to inform grid management and resilience efforts.

ARIES and HPC Scale Home Simulations for Grid Flexibility

Portland General Electric, with funding from the DOE Building Technologies Office, is working with NREL researchers to investigate advanced grid flexibility when controlling air-source heat pumps, water heaters, battery energy storage, and electric vehicles at a whole-neighborhood scale. To evaluate these new grid controls, the team is studying a simulated neighborhood representing 4,000 homes within Portland General Electric's service area. Researchers modeled the homes and developed a real-time simulation environment on Kestrel, then used NREL-developed controls, also running on Kestrel, to manage the assets. These simulations enabled NREL to ensure that their community model is ready for integration with controls in the next phase of the project: the team will deploy a commercial distributed energy resource management system (DERMS) and interface it with Portland General Electric's simulated neighborhood. The connection of commercial grid controls to simulations on the Advanced Research on Integrated Energy Systems (ARIES) platform using HPC will demonstrate how intelligent management of behind-the-meter devices can amount to megawatts of grid flexibility. By interconnecting commercial grid controls to simulations on Kestrel running in real time, researchers can study the impact at scale, enabling the utility industry to leverage these new control technologies faster and with broader impact than has previously been possible.
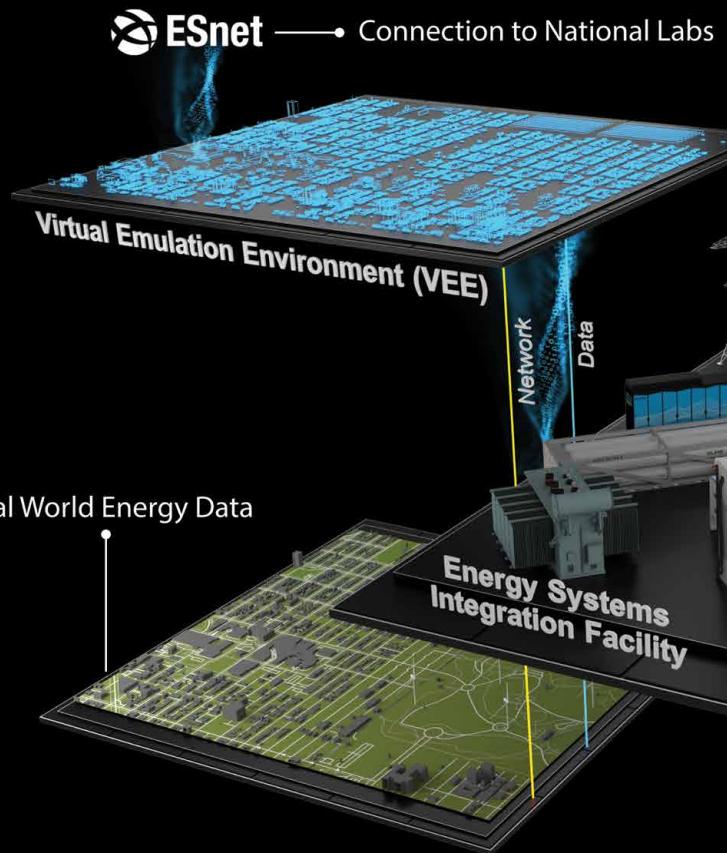
National Transmission Planning Study Defines Long-Term Planning Scenarios for a Growing Power System

The U.S. transmission system needs upgrades and expansion to accommodate energy generation and loads, and to provide reliable, affordable power to consumers. The National Transmission Planning Study (NTPS), funded by the DOE Grid Deployment Office and in partnership with NREL and Pacific Northwest National Laboratory, embarked on a multiyear quest to understand the changes needed to serve customers as the power sector evolves. NTPS seeks to identify transmission portfolios with broad-scale benefits to electric customers under a wide range of potential futures. NTPS also aims to inform planning processes for regional and interregional transmission and to identify interregional and national strategies to maintain grid reliability. New grid-scale planning tools and methods can assist industry with planning interregional transmission capacity needs. Using the Kestrel supercomputer, NTPS utilized, expanded, and created new and existing national transmission planning tools and models—the multi-model framework can help industry looking to understand transmission benefits and development options. NTPS also revealed that accelerating transmission deployment has the added benefit of reduced system costs. The six-chapter NTPS report is available from the Grid Deployment Office.
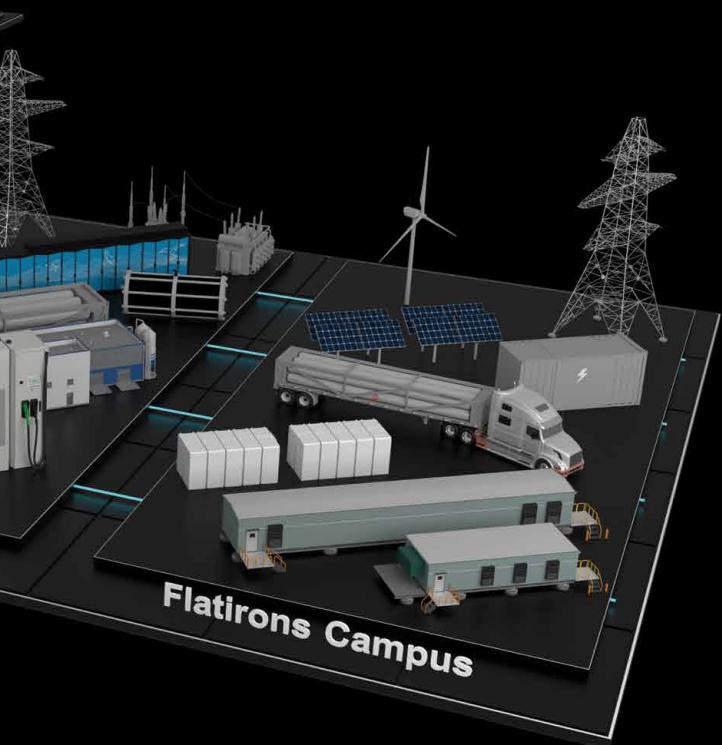
# Deep Reinforcement Learning Algorithm Stabilizes Voltage Control

Increasing energy generated through solar PV into grid distribution networks may adversely affect and tax grid operations while presenting issues in maintaining voltage stability. To address the challenges that traditional model-based control algorithms may face in this case, researchers from NREL and the University of Connecticut—with funding from the DOE Solar Energy Technologies Office—used Kestrel to develop a visibility-enhanced, model-free deep reinforcement learning algorithm. The algorithm uses surrogate models for efficient training, improving voltage regulation with minimal curtailment in distribution systems, and demonstrating scalability and real-time performance in real-world scenarios. The model-free approach allows robust regulation of voltage with limited system knowledge, enabling scalable, practical integration of distributed energy generation into power grids while accounting for grid stability. The team assessed the feasibility and effectiveness of the algorithm by testing deep reinforcement learning across varying degrees of observable data and training environments. This method paves the way for more accessible real-world applications of deep reinforcement learning and showcasing its potential to other areas of power system control.

Enhancing Wind Farm Design and Analysis Tools

The Holistic, Multi-Fidelity Wind Farm Design Optimization and Model Coordination project is funded by the DOE Wind Energy Technologies Office to advance cutting-edge multi-fidelity and systems-level methodologies for wind energy systems. In partnership with Sandia National Laboratories, Purdue University, Stanford University, and Brigham Young University, the project aims to enhance the interoperability and application of low- to mid-fidelity engineering design and analysis tools. In FY 2024, the team designed a 22-MW reference offshore wind turbine, including comprehensive design studies for the semisubmersible floater supporting the new turbine. Using aeroelastic tools from around the world—including NREL's OpenFAST wind turbine simulation tool—the team performed verification studies to validate the reference turbine. The team has demonstrated new design methodologies and innovation pathways using Kestrel for numerical simulations. By better coordinating the portfolio of numerical tools, the impact of research spans across models and fidelities, promoting broader usage in both research and industry settings. Beyond the new reference turbine, studies focused on the turbine-plant coupling and improving wind plant performance through site-customized turbine designs and control. Plant studies focused on the minimization of land-usage of wind farms and environmental impact.
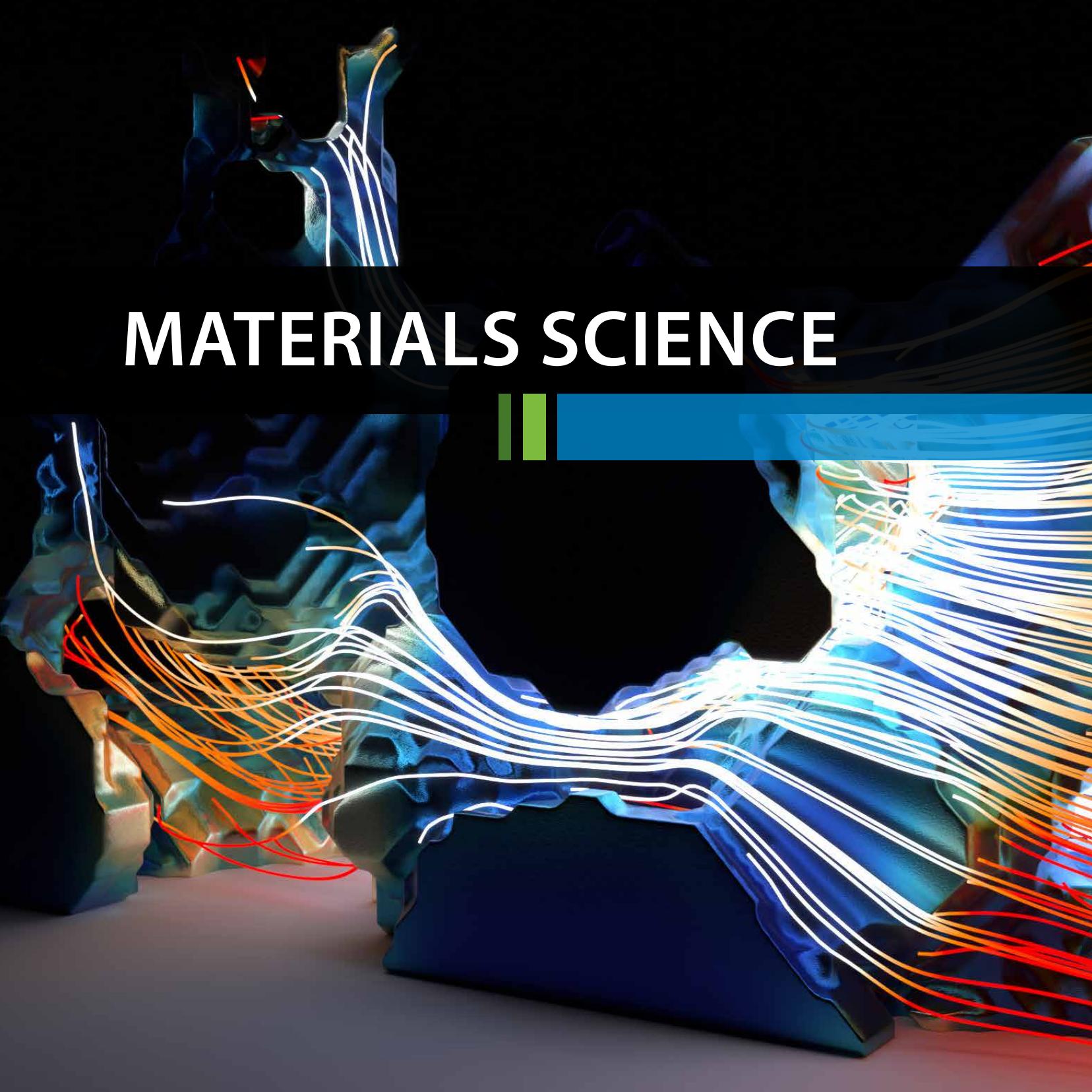
MATERIALS SCIENCE

Unlocking Better Batteries: How Tiny Atomic Patterns Boost Performance

The Cation-Disordered Rocksalt Cathode Materials Consortium is commercializing a new family of battery cathode materials: disordered rock salt (DRX). These new materials could provide higher energy density than lithium-ion battery cathodes composed of cobalt and nickel, metals with critically dwindling supply. Lithium batteries made with DRX cathodes may address supply concerns—and resulting higher prices—for the vehicle industry. Scientists found that small regions of structured order, known as "short-range order," play a crucial role in determining how well lithium ions move within the material. Using powerful imaging and simulation techniques, they identified three basic structural types—tetrahedrons, octahedrons, and cubes—within these patterns. These structures form pathways for lithium ions to travel, directly impacting the material's electrochemical performance.

With funding and support from the DOE Material Science and Engineering division in the Basic Energy Sciences program, researchers from NREL, Boise State University, and Florida State University simulated design of a new framework to map out the atomic-scale patterns of short-range order in real space, discovering that short-range order patterns correlate with lithium percolation channels and affect lithium transport properties. The Kestrel-enabled framework is based on the combination of aberration-corrected scanning transmission electron microscopy, electron diffraction, cluster-expansion Monte Carlo simulations, and simulations of scanning transmission electron microscopy imaging and electron diffraction. In addition to mapping short-range order atomic structures and matching them to lithium-transport properties, the researchers demonstrated that short-range order features can be manipulated, leading to the modification of the electrochemical performance of DRX cathodes. This discovery bridges a critical gap in understanding how local atomic structures affect battery performance and provides a roadmap for designing more efficient, next-generation energy storage solutions.

Screening Low-Cost, High-Performance Electrocatalysts and Fuel Cell Materials

Low-cost electrocatalysis is a pathway to the commercialization of hydrogen technology, but electrocatalysts have been expensive and scarce. To identify potential electrocatalysts as alternatives to noble-metal-based catalysts, researchers developed a method for screening potential electrocatalysts for the hydrogen evolution reaction and the oxygen reduction reaction. Noble metals are currently the best candidates for these reactions, so researchers aim to reduce the content of noble metals in catalysts while improving catalytic performance. Using Kestrel to perform high-throughput DFT calculations, researchers pinpointed promising candidates of low-cost, high-performance electrocatalysts and potential fuel cell materials. They additionally investigated carbon-based single-atom catalysts as alternatives to noble-metal-based catalysts for the hydrogen evolution reaction and oxygen reduction reaction. A new dataset composed of transition metals suitable for single-atom catalysts will establish physical and accessible design principles for experimentalists to use. The DOE Hydrogen and Fuel Cell Technologies Office's ElectroCat Consortium funded the work, performed by researchers from Florida State University and the University of South Carolina.
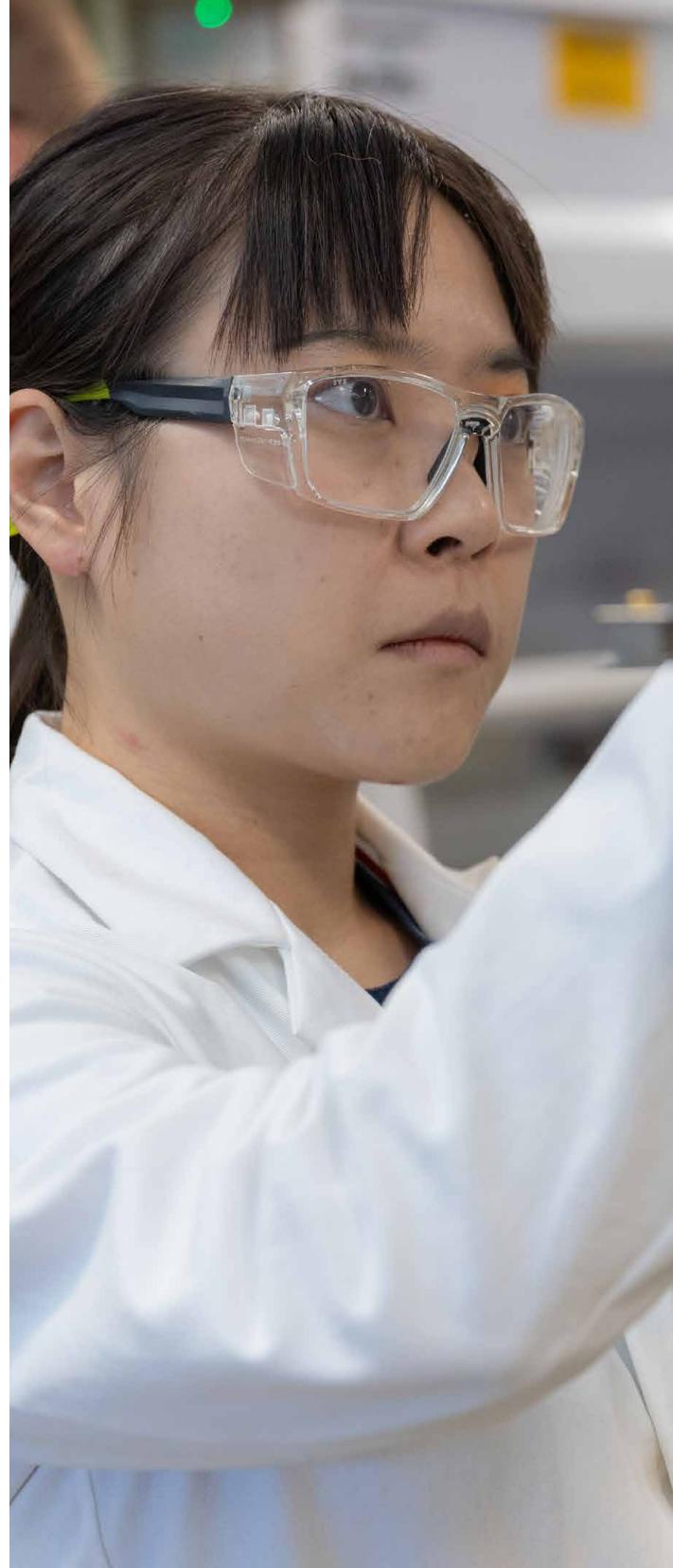
Better Understanding of Silicon Solar Cell Physics Can Improve Cell Efficiency

Silicon-based solar cells are prone to degradation, which reduces cell efficiency. Polycrystalline silicon on silicon oxide (poly-Si/SiOx) passivating contact solar cells are one of the leading candidates for high-efficiency, cost-effective, next-generation solar cells. The physics of the degradation of these tunnel oxide passivated contact (TOPCon) and polysilicon on oxide (POLO) cells are not fully understood. Researchers at the University of California, Davis developed a simulation platform, SolDeg, run on Kestrel to explore how microscopic dynamics over femtoseconds determines degradation on the timescale of decades. Adding hydrogen to the SiOx layer in low concentrations advantageously passivated the interface. This reduced recombination and thus improved cell performance. Above a critical concentration, however, excess hydrogen was found to generate pinholes that pierced the oxide layer. This dramatically increased recombination and degraded cell performance. This discovery of a sharp optimum in the hydrogen concentration is a powerful demonstration of how the SolDeg project can start on atomistic time and length scales, yet produce actionable predictions for macroscopic length and decades-long timescales.

Pathways for Enhanced Life Cycle Performance of Anodes in Lithium Metal Batteries

All-solid-state lithium metal batteries can potentially achieve both high energy density and safety, thus having received great attention. However, all-solid-state lithium metal batteries still face two major challenges: lithium dendrite growth and high interface resistance. With funding from the DOE Vehicle Technologies Office, researchers from the University of Maryland ran the first principal calculation and molecular dynamics simulations on Kestrel to establish a comprehensive criterion for effectively suppressing lithium dendrites. By utilizing simulations, the team predicted the structure and properties of various interfaces against lithium, which were then correlated with measured lithium dendrite-suppression capabilities. The simulation work conducted in this study plays a critical role in the design of solid electrolyte lithium batteries, enabling them to achieve both high energy density and long cycle life.

New Alloy Coatings Protect Hydrogen Turbine Parts

Current hydrogen turbine systems are often treated with MCrAlY (M is Ni, Co, or NiCo; Cromium, Aluminum, and Yttrium), but researchers see opportunities to enhance coatings' abilities to protect the base coatings against degradation. In FY 2024, this project worked to protect critical components in hydrogen turbine systems by taking advantage of the intrinsic merits of alumina-forming high entropy alloy-based coatings for mitigating these degradation mechanisms and offering superior oxidation and spallation resistance to the current state-of-the-art MCrAlY coatings. The team employed Kestrel and implemented an HPC-compatible model to screen new promising coating compositions with low coefficient of thermal expansion, high strength, and acceptable ductility to optimize their performance. With funding from the DOE Advanced Materials and Manufacturing Technologies Office, researchers from the National Energy Technology Laboratory worked to predict the thermal and mechanical properties of various alloys for potential use in alumina-forming, high entropy, alloy-based coatings. Modeling and validation of these alloys provided promising candidates that may help protect against hydrogen turbine system degradation.
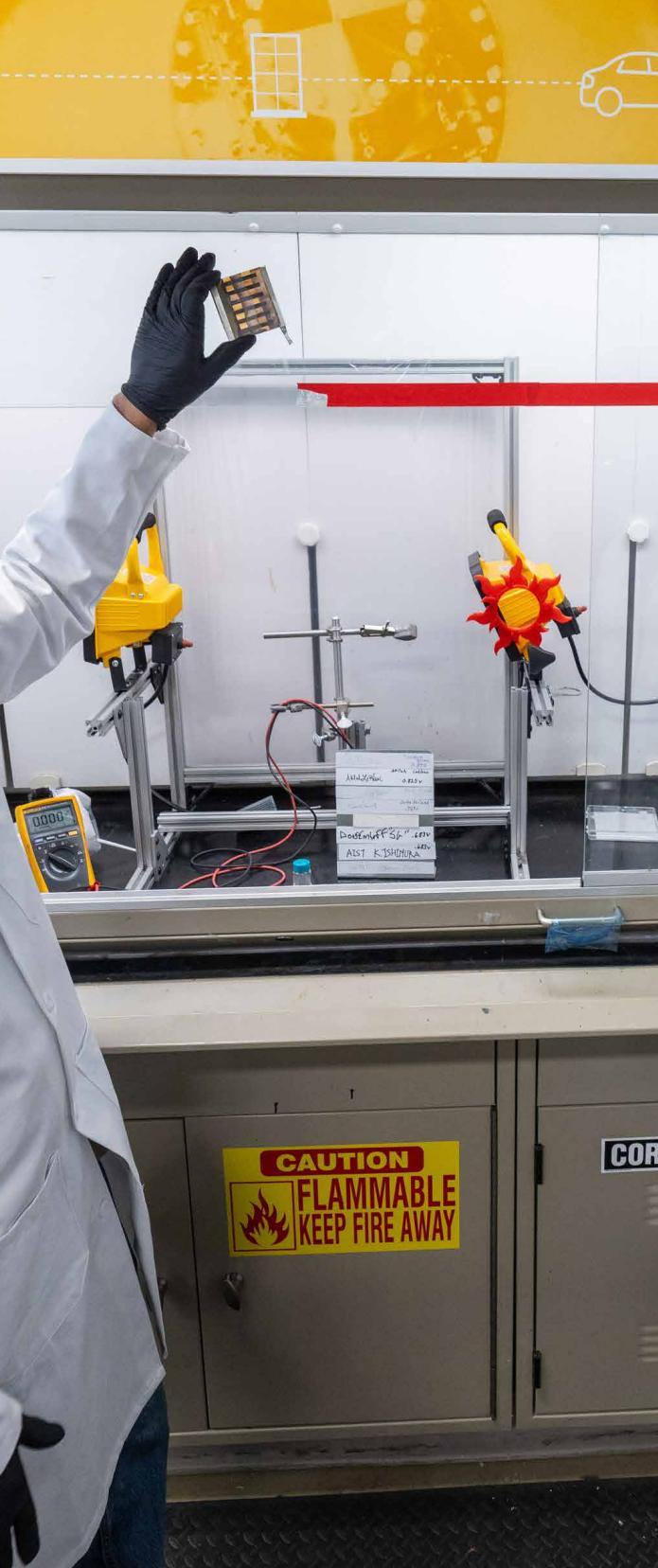
Indoor Perovskite Cell Testing Mimics Outdoor Conditions To Predict Device Stability

Metal halide perovskite solar cells (PSCs) present promising power conversion efficiency, but new technologies must show reliability under real-world outdoor conditions to reach commercialization. Stress factors like heat and humidity coexist and contribute to degradation, so NREL researchers sought to create indoor testing protocols to predict outdoor impacts and to observe related degradation in PSCs. Using Kestrel, they employed a combination of simulation and experimental methods, building a positive-intrinsic-negative PSC stack—with power conversion efficiencies of up to approximately 25.5%—and showed that indoor accelerated stability tests can predict the outcomes of 6-month outdoor aging tests. High-temperature stability tests conducted under light illumination correlated well with outdoor operational cell testing, indicating that these are key stressors to account for to understand how PSCs operate in the outdoor environment. DFT calculations and electrochemical measurements showed that enhancing the ion-blocking properties of the self-assembled monolayer hole transport layer—the site of a critical instability mechanism in PSCs—is critical for improving device stability under high temperatures in the sun. Funding for the project was partially provided by the Center for Hybrid Organic–Inorganic Semiconductors for Energy, a DOE Office of Science Energy Frontier Research Center.

Simulations Detail Properties of Lithium-Excess Rock Salt for Energy-Efficient Batteries

Lithium-ion batteries present the practical energy density needed to provide electric vehicles with a range and life cycle comparable to combustion-engine vehicles. The discovery of DRX materials provides high energy density in addition to a promising pathway to addressing resource constraints associated with cobalt and nickel, key components of traditional lithium-ion batteries. To support higher performance and lower-cost lithium-ion batteries for electric vehicles, researchers from Lawrence Berkeley National Laboratory and the University of California, Berkeley, with funding from the DOE Vehicle Technologies Office, used Kestrel and Swift—an HPC system dedicated to projects funded by the Vehicle Technologies Office—to study the electrochemical properties of DRX and partially disordered spinel-based cathodes. The researchers realized two milestones in FY 2024: the synthesis of high-performance partially disordered spinel-based cathodes; and an advanced ML technique for predicting electrochemical behaviors of cathode materials. Simulation efforts are corroborated by experiments that show improved performance of disordered cathodes. Next, researchers will continue efforts to understand design handles for controlling the DRX-to-spinel ordering transitions and investigating synthesis routes that optimize such spinel-like partial order for better performance.
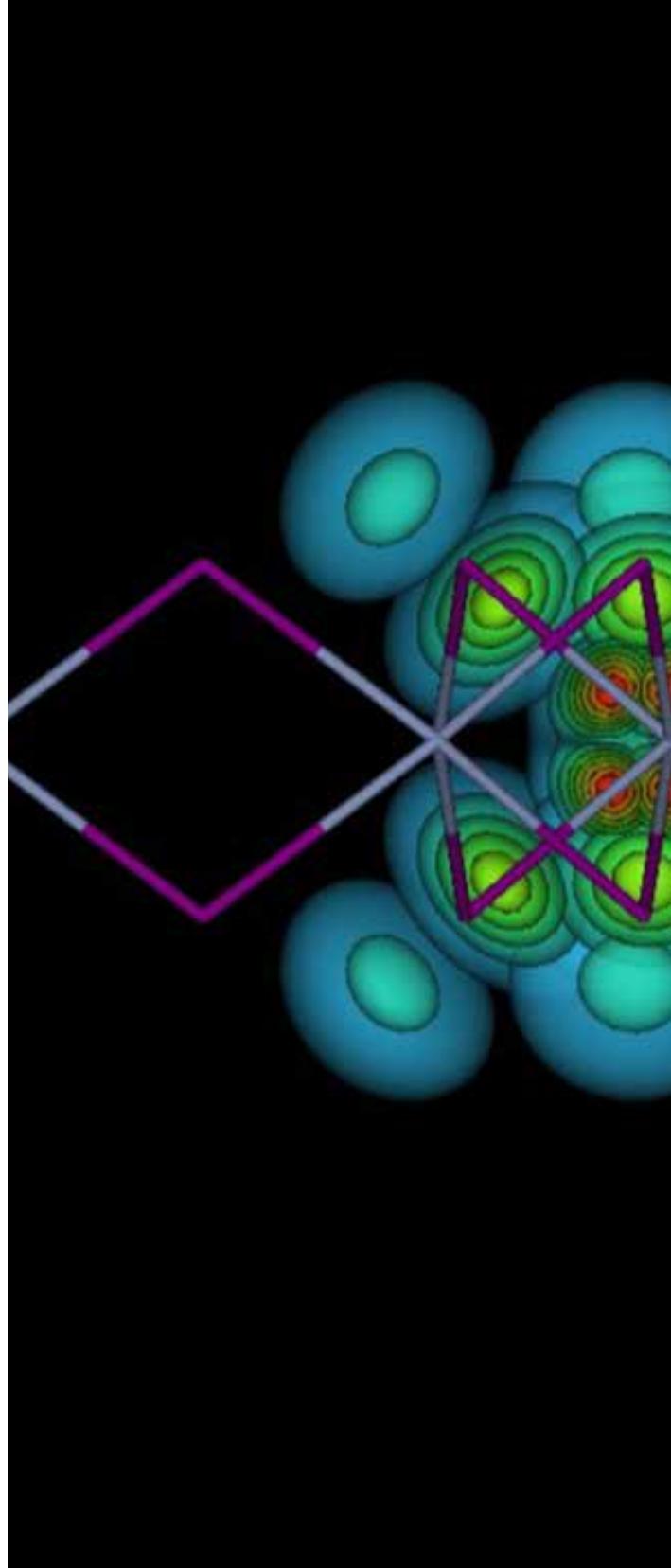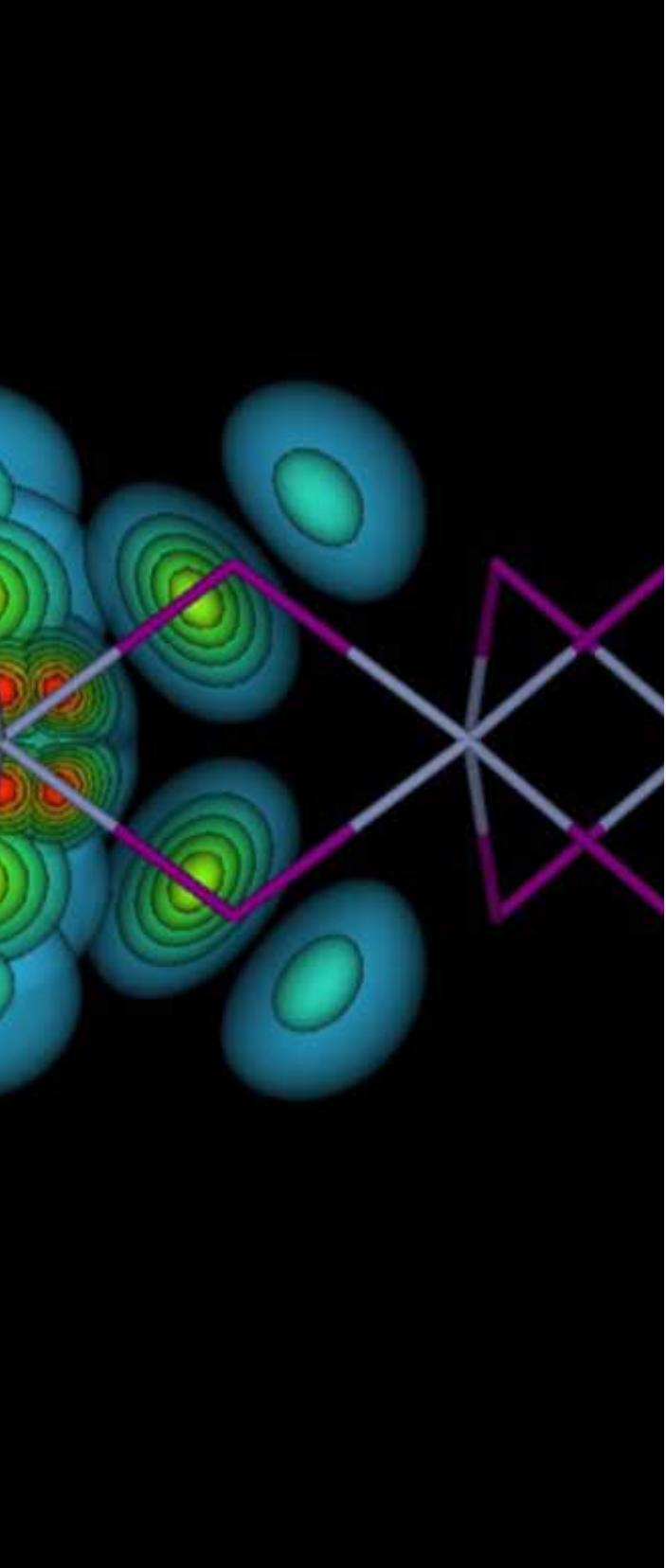
Questaal Software Resolves Complex Physics, Helping Researchers Solve Complex Problems

Questaal—a suite of electronic structure software designed to answer basic questions about chemical and solid-state systems at the atomic level—solves quantum physics equations using Feynman diagrams efficiently, simplifying computationally intensive processes enough to make it tractable but still retaining high fidelity. In FY 2024, NREL researchers used Kestrel to investigate titanium diselenide ($TiSe_2$)—thought to be a rare instance of an excitonic insulator—finding that $TiSe_2$ is not an excitonic insulator but a band insulator that appears when dynamical nuclear fluctuations are considered. Knowledge of the electronic structure is an essential prerequisite for investigating other properties of $TiSe_2$ like its superconductivity. Questaal's high fidelity, which can include excitonic effects, enables it to resolve many properties such as the optical bandgap in $TiSe_2$, where prior theories have been inadequate. This showcases Questaal's ability to answer key science questions in a wide range of studies of chemical and materials systems. In other FY 2024 projects, Questaal was used to investigate magnetic metals and their interfaces to explore the properties of LK-99 as a possible superconductor; explain many properties of excitons in recently discovered 2D ferromagnetics; investigate optical properties of carbon monoxide on a copper substrate (for catalysis); gain a basic understanding of the origin of the metal-insulator transition rare earth nickelates of interest for neuromorphic computing; explore processes in iron/magnesium oxide (Fe/MgO) tunnel junctions used in the electronics industry; and explain the core physical properties of YFe_2Ge_2, a superconductor that may support Majorana fermions.

First Macromolecular Model of Woody Plant Cell Walls Will Improve Biomass Conversion

Deconstruction of plant cell walls is the first step of the biomass conversion process, but deconstruction is expensive and energy-intensive due to the robust nanoscale architecture and strong adhesion between the constitutive biopolymers. Funded by the DOE Bioenergy Technologies Office, researchers deployed a multidisciplinary approach—including using solid-state nuclear magnetic resonance imaging to infer details about the structure—to define the macromolecular arrangement of polymers in *Populus* wood before using Kestrel to develop molecular models of the lignocellulosic biopolymer assemblies. Lignocellulosic biomass holds great potential as a source for fuels, chemicals, and materials. The models helped researchers identify which biopolymer interactions are responsible for the chemo-mechanical resilience of biomass. A molecular-level understanding of the architecture of biomass helps elucidate structure/property relationships that inform design and optimization of pretreatment strategies to reduce energy input and maximize conversion performance of the material. This project resulted in the first macromolecular model for woody plant cell walls. Though limited to a single plant species, methods can be applied to other important bioenergy crops in various states throughout preprocessing and conversion.
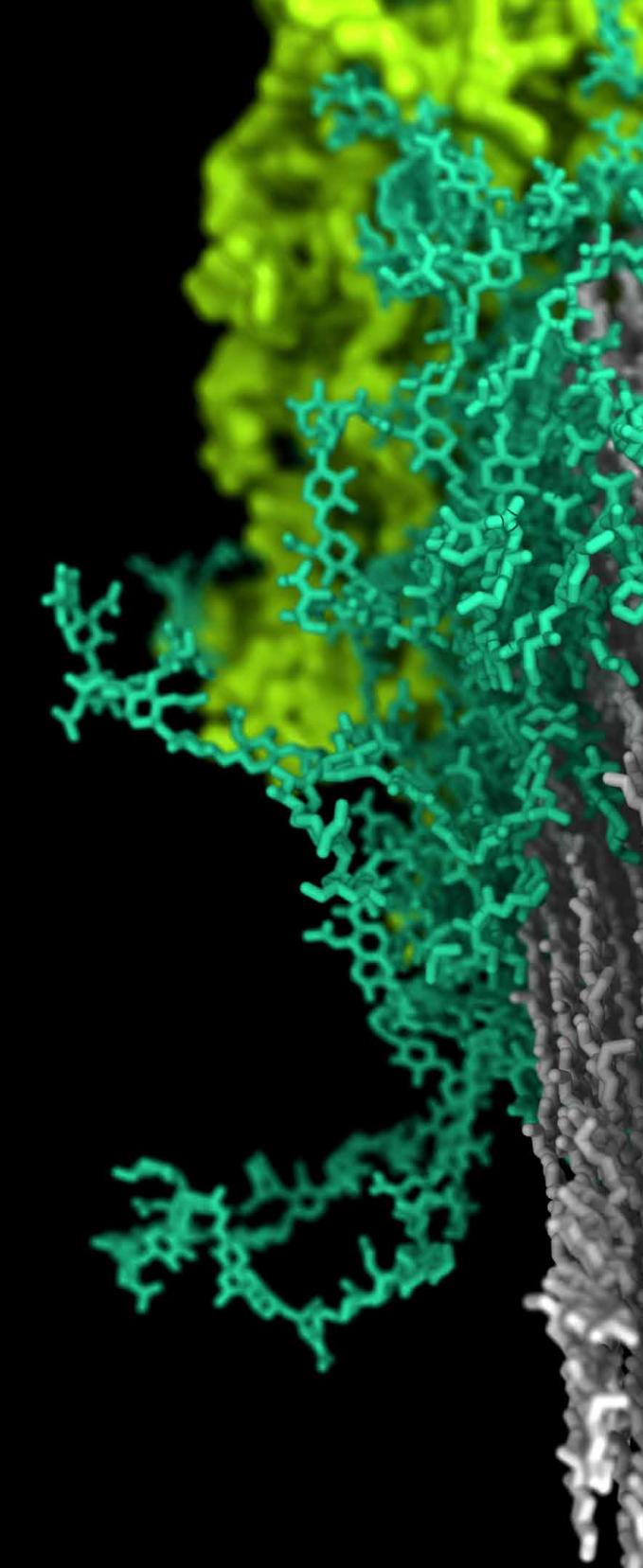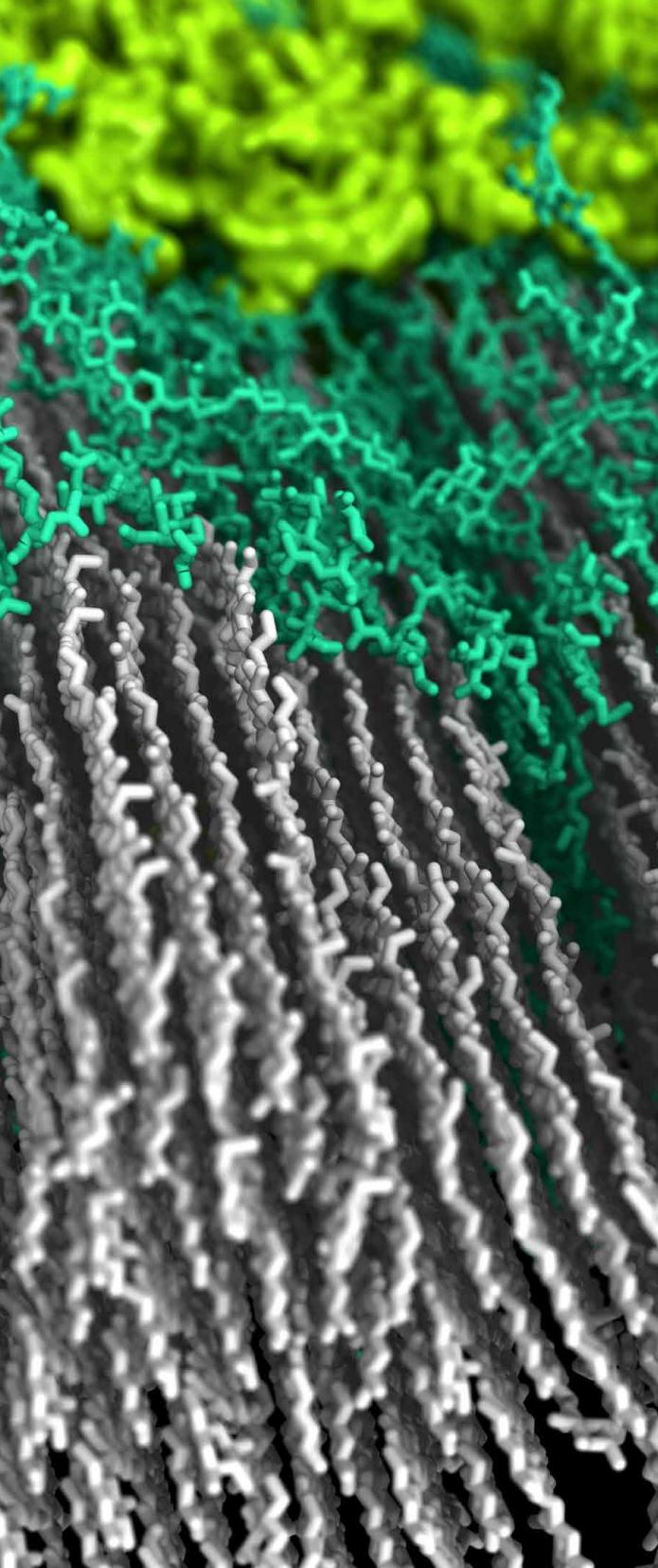
Boosting Hydrogen Cells: How To Stop Strontium From Slowing Them Down

High-temperature electrolysis using solid-oxide electrolyzer cells is a highly promising method to produce hydrogen with the help of nuclear or geothermal heat sources. These devices typically rely on a solid electrolyte material that shuttles oxygen ions at high temperatures as part of a process that splits water molecules and siphons off the hydrogen fuel. However, during operation, strontium (Sr) atoms can migrate into different layers of the cell near the solid electrolyte, forming unwanted byproducts that can reduce the device's performance by blocking the desired flow of oxygen ions. With funding from the DOE Hydrogen and Fuel Cell Technologies Office's H_2NEW consortium, advanced quantum atomistic simulations were performed to investigate how and when these Sr-containing byproducts form, how to avoid them, and what their consequences on performance might be. Based on extensive static and dynamics simulations across a wide variety of operation scenarios and cell chemistries, the team identified one compound (SrO) that was predicted to be particularly problematic. Another compound ($SrZrO_3$) was also identified as a possible issue, but the team discovered that even trace quantities of yttrium, which is found naturally in certain parts of the solid-oxide electrolyzer cell, can mitigate these drawbacks. The research team, with contributors from Lawrence Livermore National Laboratory and NREL, used the Kestrel supercomputer to perform these high-fidelity calculations and combined the results with experimental validation. In addition to elucidating key mechanisms of Sr-associated performance loss in solid-oxide electrolyzer cells, the results point to ways solid-oxide electrolyzer cell synthesis and cell designs could be modified for improved lifetimes.

Amorphization Modeling Yields Design Insights for Ultrawide Bandgap Material Design

Aluminum nitride (AlN)-based alloys are ultrawide bandgap materials used for optoelectronics and electromechanics. Researchers have modeled alloys assuming the existence of crystalline phases only. However, alloy thin films when synthesized in a laboratory are sometimes amorphous (i.e., they lack well-defined crystal structures). Consequently, certain alloy compositions cannot be synthesized as crystalline phases. Crystalline and amorphous phases generally exhibit significantly different functional and mechanical properties. Thus, it is crucial to accurately predict the alloy phase diagram. With funding from the Basic Energy Sciences program within the DOE Office of Science, researchers ran molecular dynamics on Kestrel to simulate amorphous (Al,RE)N heterostructural alloys (RE are rare-earth elements like gadolinium and terbium) and precisely mapped the alloy compositions prone to amorphization when synthesized. They showed that the tendency to amorphize is related to the fundamental elemental properties of aluminum and RE—a materials design guideline to inform the selection of elements to alloy depending on whether crystalline or amorphous alloys are desired. Developing new ultrawide bandgap (aluminum,gadolinium)N alloys that are monolithically integrated with microelectronics to enable neutron detection has potential for applications in particle physics, radiation safety, and homeland security.

MANUFACTURING

More Resilient Polymer Membrane Options for Scalable Water and Biofuel Filtration

Organic solvent nanofiltration (OSN) is an emerging separation technology that uses a porous membrane to selectively filter undesired molecules out of a liquid (i.e., solvent). OSN's energy efficiency and scalability for industrial applications make it a promising option to purify water, biofuels, and hydrogen, and assist in carbon capture of industrial emissions. However, current OSN membranes are susceptible to degradation and not stable enough for recurring use. With funding from the DOE Industrial Technologies Office National Alliance for Water Innovation, researchers from the University of Connecticut used the Kestrel supercomputer to model the resiliency of polymeric membranes for OSN. Researchers combined theoretical modeling, nonequilibrium molecular dynamics simulations, and experimental data to create a solution-friction model. Using this model, accurate and computationally efficient forcefields were identified, enabling ML combined with nonequilibrium molecular dynamics simulations to explore the desalination performance of approximately 1,000 polyamide membranes. The major discovery from the solution-friction model is that the successful transport of solvent mixtures through a polymeric membrane occurs due to the pressure differences on either side of the membrane, rather than the concentration levels of the different substances in the mixture. This research indicates that OSN membrane design should focus on controlling the pore architecture, not the solubility of solvents.

Simulations Reveal Energy-Efficient Steelmaking Reduction Pathway

Steelmaking emissions originate primarily from carbon-intense industrial heat and coke-based reduction that drive the iron ore reduction process. Hydrogen plasma smelting reduction is a promising new technology that can improve steelmaking with the use of hydrogen and electricity, but the process creates extreme environments with high temperatures, utilizes capital-intensive equipment and operations, and presents scale-up challenges. Researchers used Kestrel to develop a first-principles continuum-scale model for argon/hydrogen thermal plasmas used in hydrogen plasma smelting reduction, which was presented recently at the 2024 American Chemical Society fall meeting. Plasma modeling showed that the addition of hydrogen results in a diffuse plasma and lower temperatures from higher thermal diffusivity of hydrogen compared to pure argon. Coupled reaction and transport models showed that the rate at which hydrogen moves through the porous ore is the main factor limiting how quickly ore is reduced. These simulation insights will accelerate the transition of the steel industry without the need for expensive experimental testing.

Simulations Inform 3D Printing of Ultra-High-Temperature Parts for Better Gas Turbines

Gas turbines need materials that can handle extremely high temperatures—over 1,300°C—to improve efficiency. Refractory metal alloys like C103 work well under these conditions. The Commonwealth Center for Advanced Manufacturing and Oak Ridge National Laboratory are studying how to 3D print C103 parts by testing different printer settings—such as laser power and scanning speed—and using computer simulations on Kestrel and the HPC systems at Oak Ridge to see how the metal behaves and solidifies. The simulation framework supports the optimization of the powder direct energy deposition advanced manufacturing process to reduce design lead time and minimize rejected parts or raw material consumption. By running these simulations on powerful supercomputers, the team can fine-tune the manufacturing process to make stronger parts faster, reduce waste, and speed up development for next-generation gas turbines.
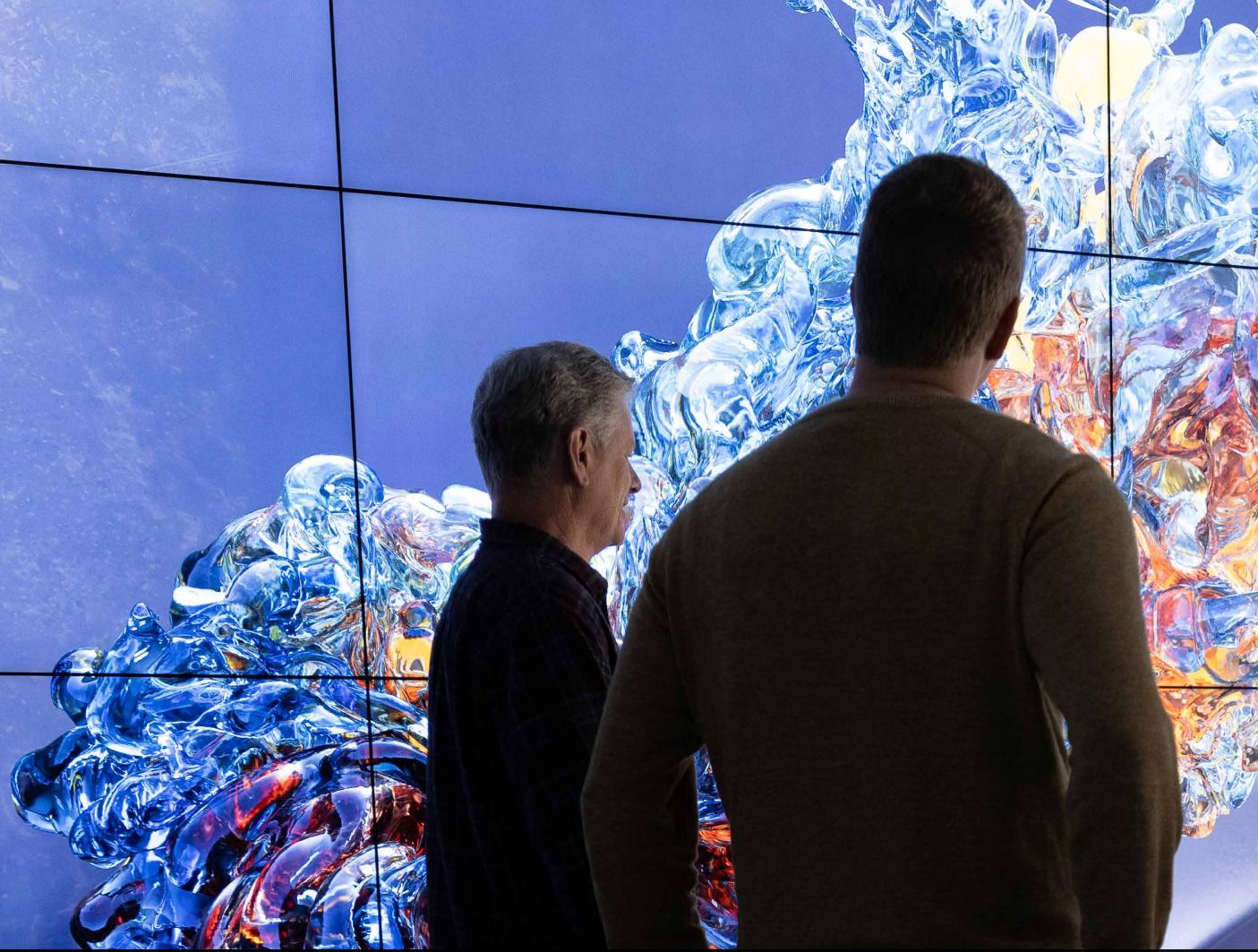
FLUID DYNAMICS

Timing and Direction of Powerful Vibrations Can Prevent Biomass Clogs in Mill Equipment

The variability and high degree of cohesiveness in common biomass feedstocks can severely reduce their flowability, leading to clogging of biorefinery machinery, and has been highlighted as one of the central challenges in the handling and conversion of biomass. While experimental techniques can shed some light on strategies for improving biomass flowability, such approaches are generally limited to small-scale configurations that are not necessarily applicable to industrial-scale applications. Numerical modeling is thus an invaluable tool for gaining insight into strategies for handling milled biomass feedstocks. As part of the DOE Bioenergy Technologies Office-funded Feedstock-Conversion Interface Consortium, researchers from NREL simulated biomass flow behavior using Kestrel. They focused on developing a high-fidelity, high-performance framework for simulating biomass flow through biorefinery equipment, and developed an open-source library. Researchers used the model to investigate how vibrational forcing techniques can help improve flowability, and gained insight into how the forcing amplitude, frequency, and direction can help feedstock discharge from a wedge hopper. This results in further understanding of the physical processes involved in biomass feedstock flowability and feedstock handling, contributing to the scale-up and start-up of demonstration and commercial-scale biorefineries.

AI Algorithm Blends Atmospheric Measurements With Physics-Rich Simulation Data

The Rotor Aerodynamics, Aeroelastics, and Wake (RAAW) project advances our understanding of atmospheric measurements critical for wind energy, air quality, and wildfire research. While atmospheric field campaigns provide essential data, practical constraints often limit sensor deployment, resulting in measurements from only unevenly distributed locations. Although physics-based computational models can help extrapolate atmospheric dynamics from measured to unmeasured regions, previous approaches relied on simplified models that overlooked crucial physical processes. To address this limitation, NREL researchers, supported by the DOE Wind Energy Technologies Office, developed an innovative ML approach that leverages large-eddy simulation, an advanced atmospheric modeling technique. This methodology enables the reconstruction of wind speeds across an entire turbine rotor disk using measurements from the turbine hub height. By providing a comprehensive view of wind patterns across the rotor disk, researchers can better analyze how spatial wind variations influence turbine structural responses. This enhanced atmospheric reconstruction capability complements the ExaWind simulation framework, enabling more rigorous validation of aerodynamic and structural models for modern wind turbines, which in turn, provides turbine manufacturers more confidence when designing next-generation turbines.
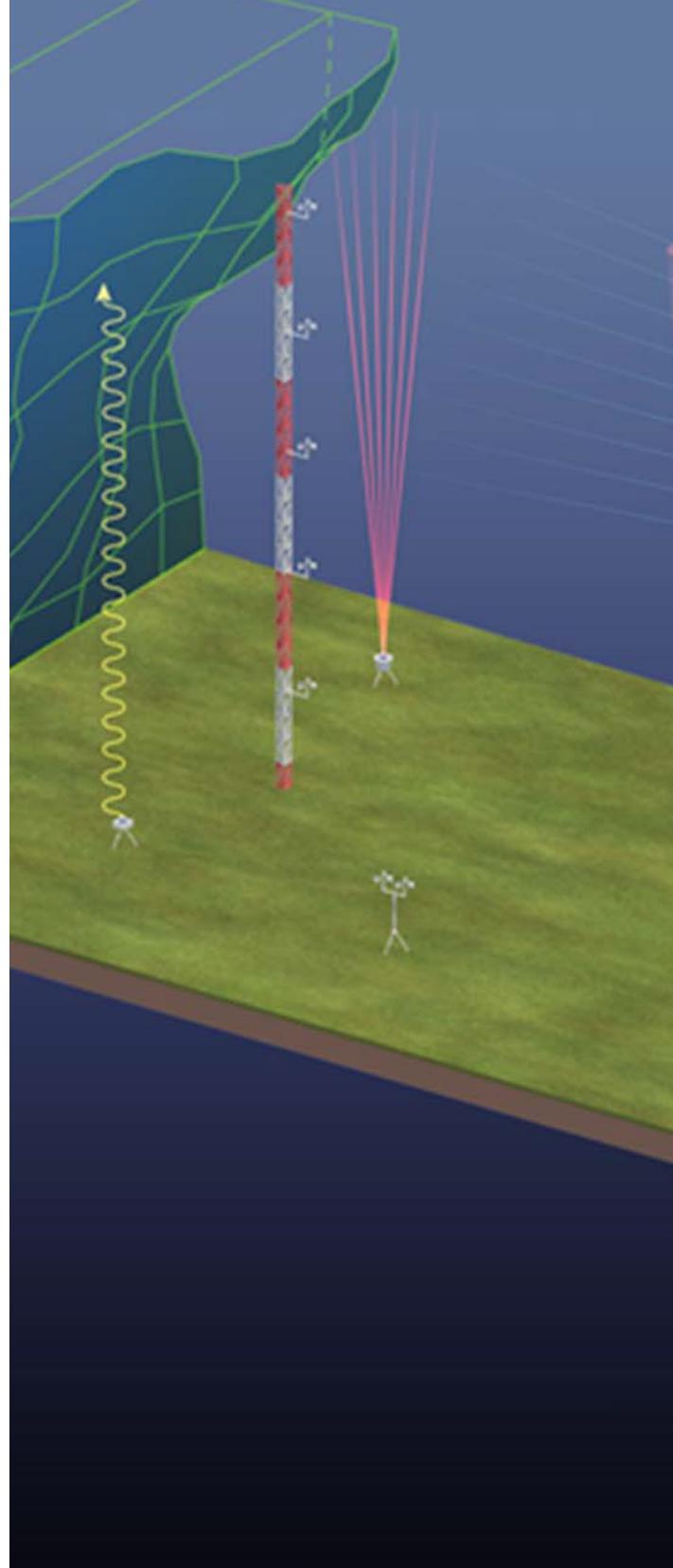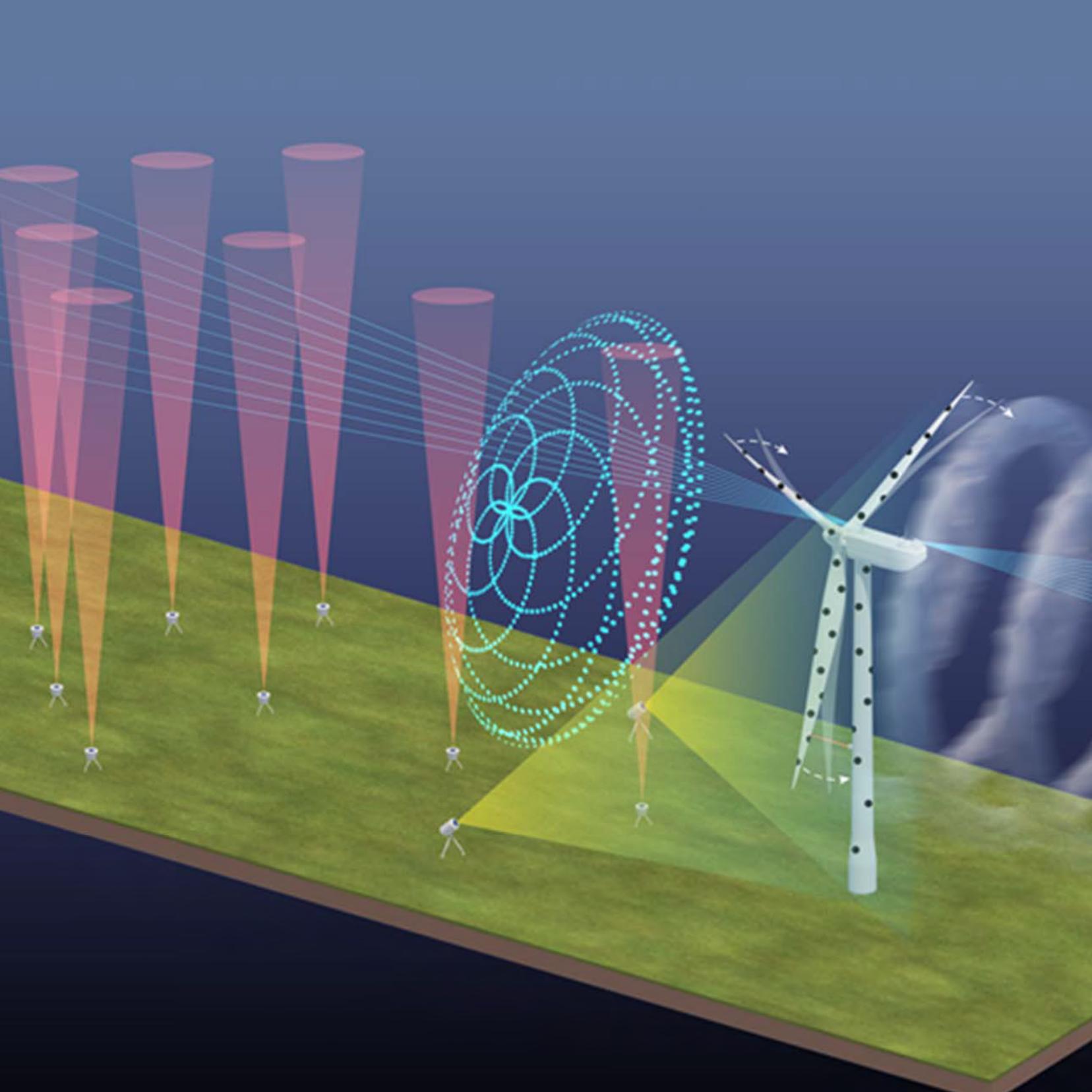
Harnessing Energy Data for Resource Assessments

Growing interest in wave, tidal, current, ocean thermal, and river energy potential has advanced the need for accurate, diverse, and high-resolution datasets. Funded by the DOE Water Power Technologies Office, researchers from Pacific Northwest National Laboratory, Sandia National Laboratories, and NREL utilized Kestrel to simulate and process marine energy models and to expand publicly-available high-resolution datasets using WaveWatch3 and Simulating WAves Nearshore (SWAN) wave modeling software. One example of these modeling efforts includes the production of year-long, high-resolution datasets (e.g., ~100 meters) for tidal energy priority sites in the United States (e.g., Cook Inlet and Puget Sound). Data supported by Kestrel is continuously being disseminated through NREL's Marine Energy Atlas, which supports the assessment and selection of deployment test sites, supports engineering requirements definition, and provides valuable information about options to diversify energy sources and increase energy resilience.
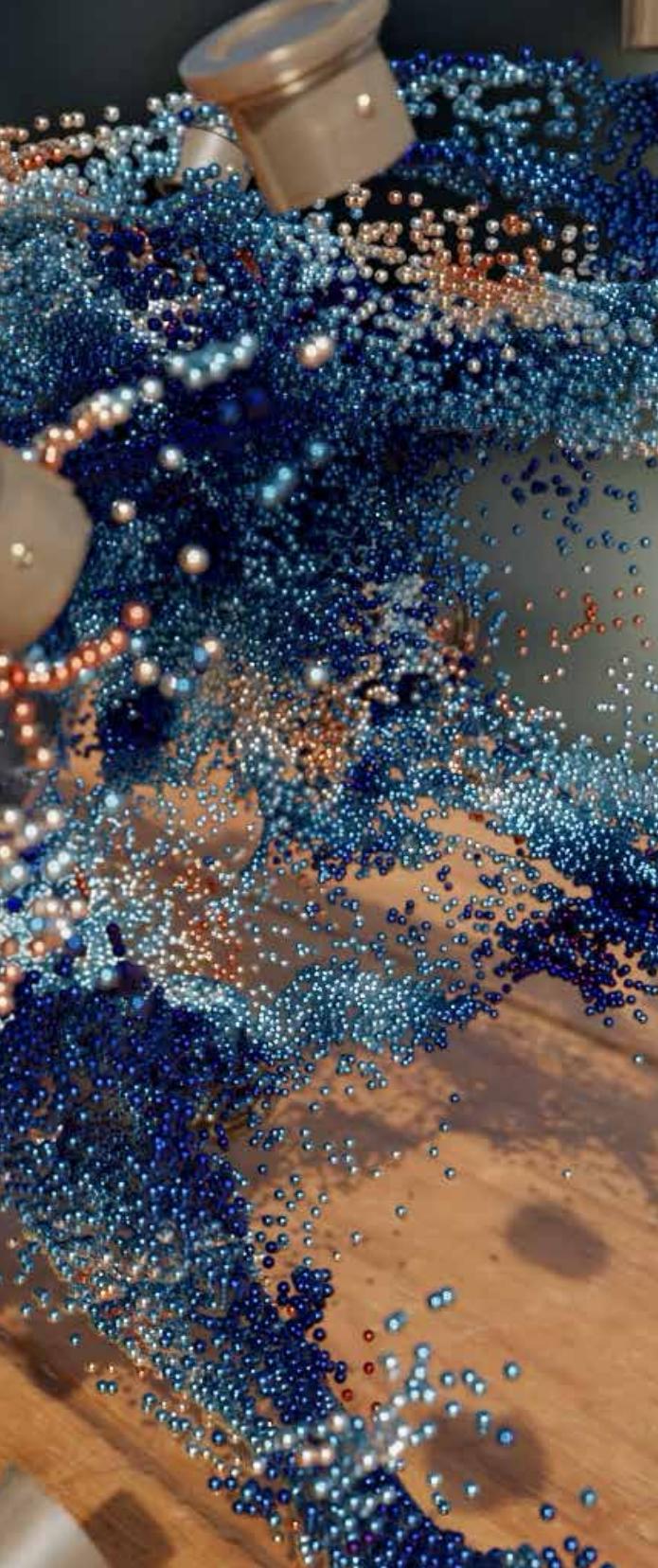
Investigating Biofuel and Engine Design To Advance Fuel Efficiency

A new need has emerged for engines designed for bioblendstocks—biofuels blended with fossil fuels—that ensure maximum fuel efficiency and minimal pollutant emissions. To help the vehicle sector optimize bioblendstock and engine designs, NREL researchers are using chemical kinetic models to evaluate fuel performance at a molecular level. These models help researchers determine the most favorable combustion conditions (e.g., temperature, pressure, and mixing rate) for a given bioblendstock. With DOE Vehicle Technologies Office funding, NREL researchers used Kestrel to simulate performance of several candidate bioblendstocks at various operating conditions inside its Advanced Fuel Ignition Delay Analyzer—a combustion chamber. These computational fluid dynamics (CFD) simulations focused on investigating ignition times and nitrogen oxide emissions. Measurements of fuel properties critical to engine performance were calculated at extreme operating conditions (e.g., very low or very high temperatures and pressures). The experimental data gleaned from these simulations are helping researchers develop combustion kinetic models for different bioblendstocks, enabling multiple mobility sectors to leverage improved fuel efficiency for alternative liquid fuels.
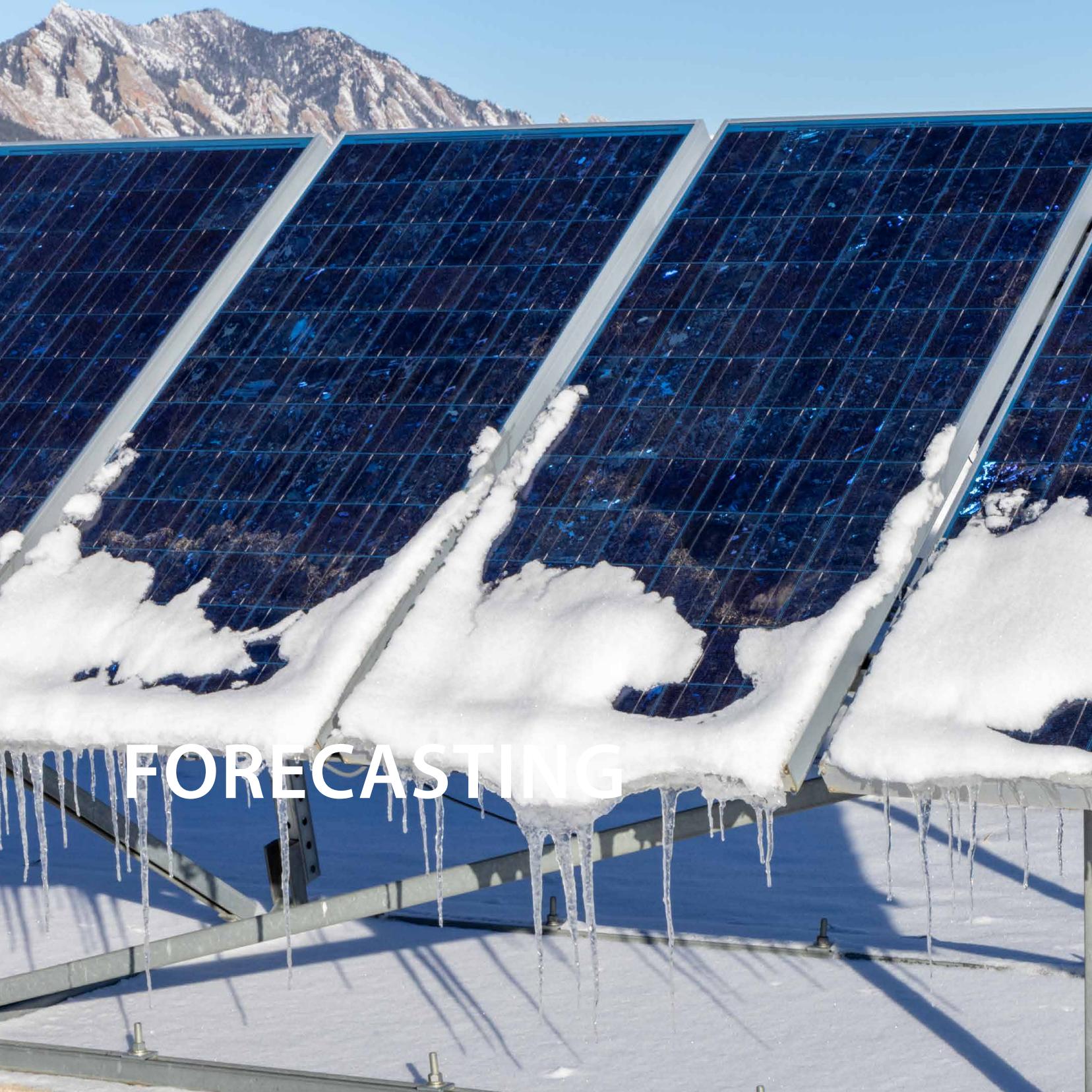
FORECASTING

Enhancing Energy Sector Readiness for Extreme Weather Events

The Energy System Planning for Resilience During Severe Weather (ESPRSW) project aims to improve the energy sector's ability to manage, ensure resource adequacy, and plan for the impact of severe weather on future energy systems by integrating methodologies such as climate data downscaling, energy generation modeling, and power system operational analysis. Increasing occurrence of severe weather events poses significant risks to energy system planning and operations, and incorporating these factors into planning tools is complex. The energy sector currently lacks a common set of tools or guiding principles for managing these risks. To use generative ML to downscale climate data, we must ensure that models are trained on data with sufficient information across scales, from large spatiotemporal scales of input climate models to small scales of state-of-the-art historical meteorological datasets. Previous models trained on Eagle struggled with a small effective receptive field that limited the ability to preserve cohesive weather patterns across multiple days. Using Kestrel's new H100 GPUs, the research team designed new model architectures with larger effective receptive fields that greatly improve the quality of the downscaled climate data. These improvements will be present in the new Sup3rCC v0.2.2 datasets, to be released in 2025.

Coupled Simulations Reduce Uncertainty for Energy Production

The 3rd Wind Forecast Improvement Project (WFIP3), sponsored by the DOE Wind Energy Technologies Office, aims to enhance the understanding of atmospheric and ocean physics affecting offshore wind resources along the U.S. East Coast. Researchers used Kestrel for atmospheric and coupled ocean/wave/atmospheric modeling, showing the sensitivity of wind and turbulence to factors like turbulence parameterizations, initial conditions, land-sea circulations, wind/wave interaction, and hypothetical wind wakes. These multiyear simulations highlight the importance of three-way coupling between wind, ocean, and waves, reducing uncertainty in wind speeds near surface and improving wave height predictions, especially off the northeastern U.S. Atlantic Coast. High-resolution ocean temperature data further refine these models.

Parameterization of theoretical wind farm wakes in high-resolution revealed sea surface warming patterns around the major wind energy lease areas under stably stratified atmosphere-ocean boundary layer conditions. By quantifying the influence of wind farms on coastal upwelling and mixed-layer dynamics, this research can inform strategies for optimizing energy production while minimizing potential ecological disruptions.
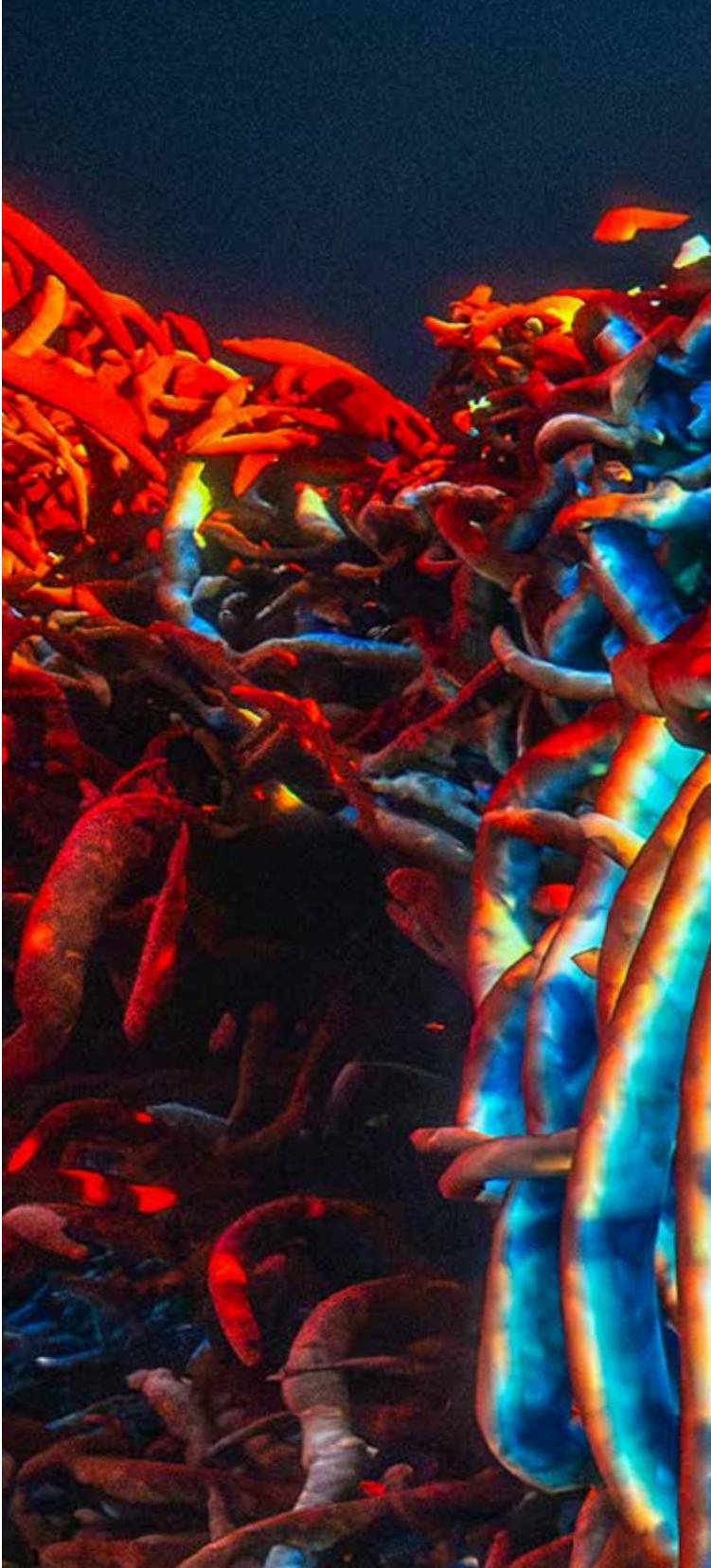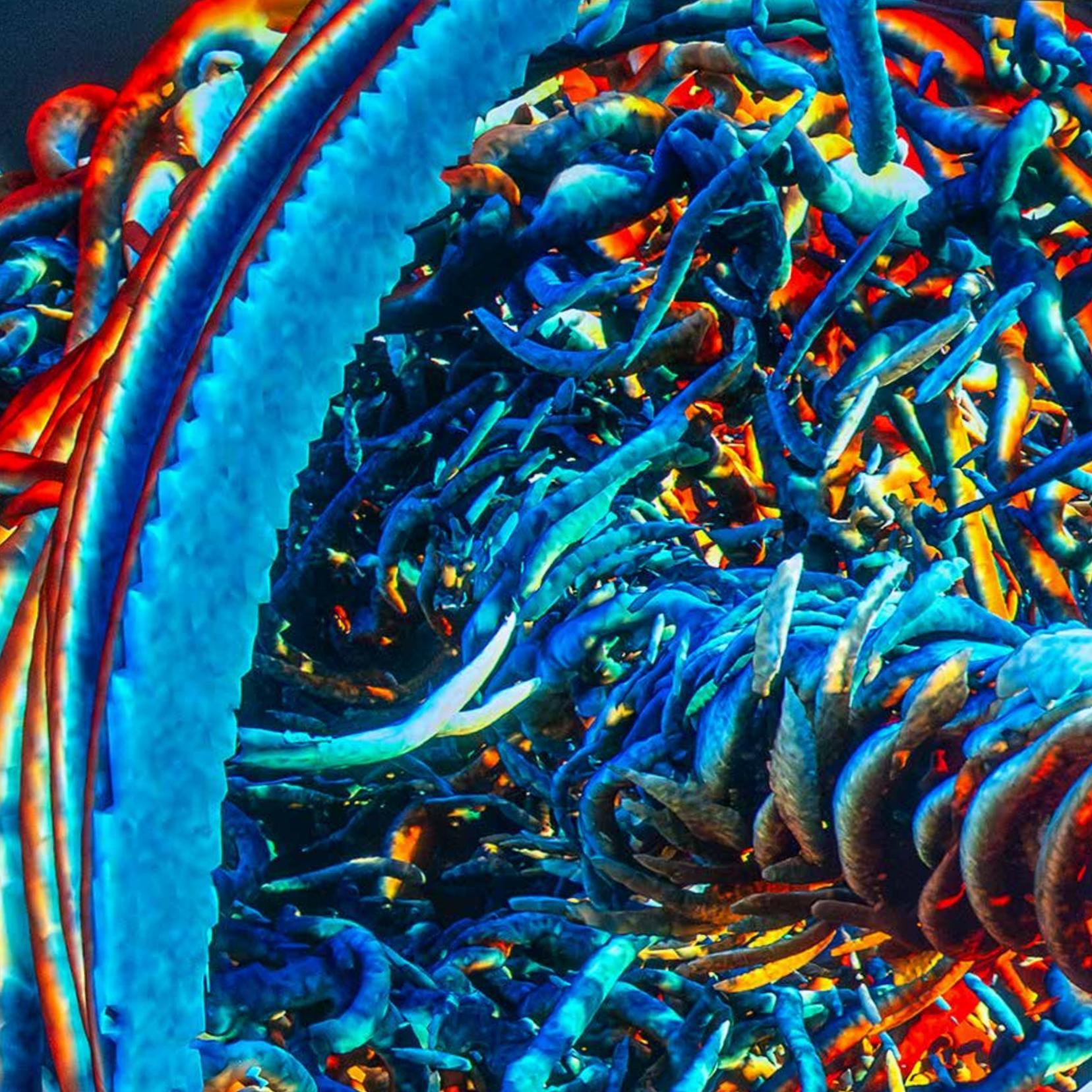
A BROADER COMPUTING ECOSYSTEM

NREL has a compute solution for every research task, where projects often require integrating commercial and on-premise cloud services with the HPC system to support the breadth of research projects across DOE and partners. NREL's Stratus Cloud Team enables commercial cloud solutions by partnering with Amazon Web Services, Google Cloud, and Microsoft Azure, and supports more than 175 projects. NREL's on-premises cloud computing system includes both GPU and CPU resources, tied together with an on-demand cloud-based job scheduler. The integration of these multiple compute capabilities creates a broader computing ecosystem, a growing part of the computational capabilities hosted at NREL.

Tool Enables Evaluation of Perovskite Solar Cells

As part of the Photovoltaic Accelerator for Commercializing Technologies (PACT) project, researchers needed access to detailed time series and voltage-current curves from experimental PV device data. The PV current voltage database (PVIVDB), hosted in the cloud, collects experimental data from PV modules, including outdoor and indoor current-voltage characteristics, operating point, temperature, incident irradiance, and ambient temperature. The tool is flexible and adaptable, handling new and emerging data for new experiments. Understanding PV module performance and how it changes over time in a variety of conditions is critical to accurately predict their long-term energy yield. The PVIVDB was particularly useful this year when researchers examined how metal halide PSCs' degradation mechanisms work under outdoor conditions. The team recognized that many indoor tests of PSCs using light-emitting diodes do not expose them to the levels of ultraviolet (UV) light radiation they would receive outdoors. Therefore, it is important to understand the degradation mechanisms in these cells in sunlight and associated UV. Using the PVIVDB to collect performance data of PSCs operating outdoors, researchers investigated degradation mechanisms in positive-intrinsic-negative-structured PSCs to further understand the differences in indoor and outdoor durability. They found that faster degradation occurs in the perovskite/indium-tin oxide interface, leading to new material designs for high efficiency and improved UV stability of perovskite devices.

Improved Analysis and Reporting of PV Field Performance

NREL researchers convened to examine an ambitious pathway for degradation science. Aggregating data from multiple sources, performing rigorous analysis, and making public the lessons learned can often be difficult due to the proprietary nature of performance data. Facing this need for aggregated, available data to serve degradation science, the PV Fleet team has built the Photovoltaic Durability and Reliability Database (PVDRDB), hosted in the cloud and deployed on Amazon Web Services Redshift, which demonstrates the possibility of aggregating proprietary data, performing analysis (on Kestrel), and communicating key lessons, all of which has informed this project going forward. PVDRDB hosts, in the cloud, high-quality commercial and utility-scale PV systems data with an average lifespan of 5 years at 15-minute data resolution. There are approximately 9 GW of deployed sites included, which represent 10% of the U.S. PV commercial and utility fleet. The availability and aggregation of data will help NREL degradation researchers perform fundamental science that can advance the energy efficiency of key technologies.
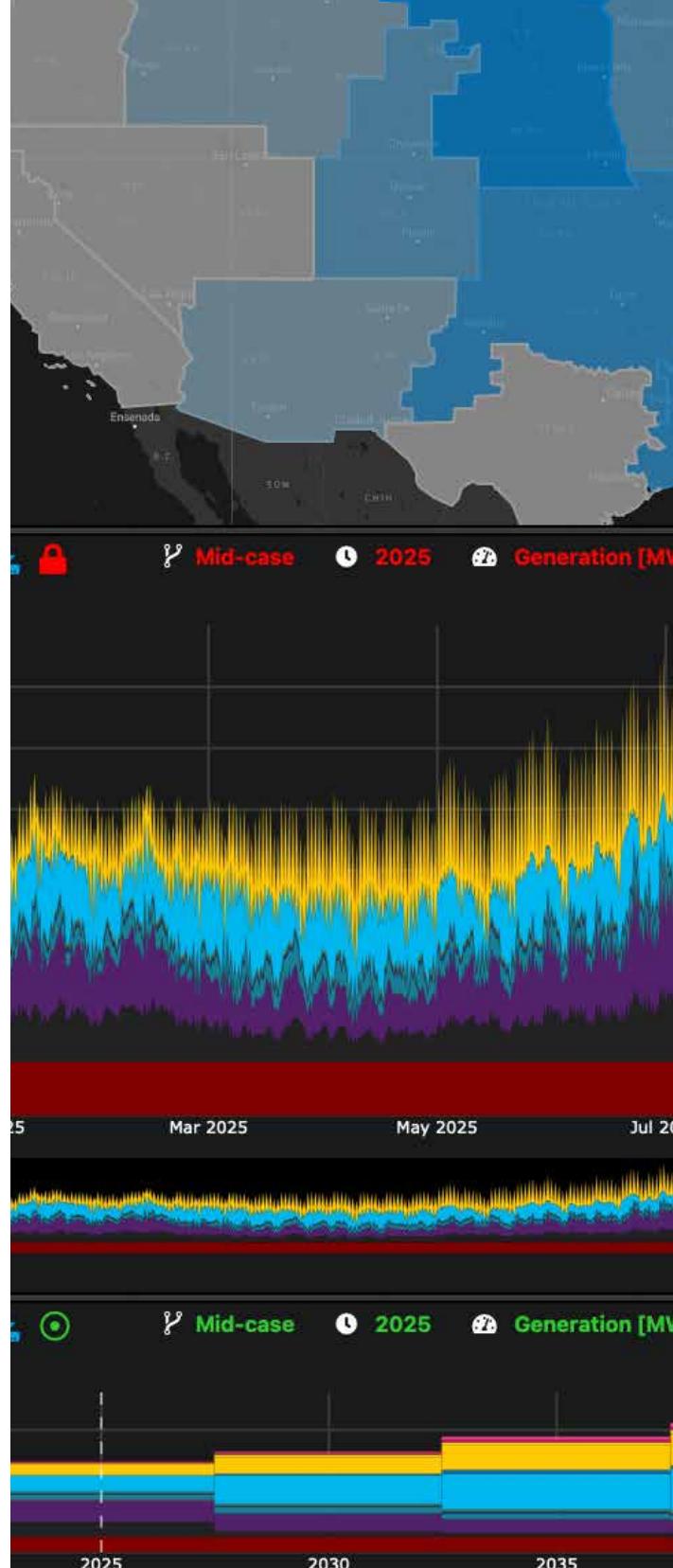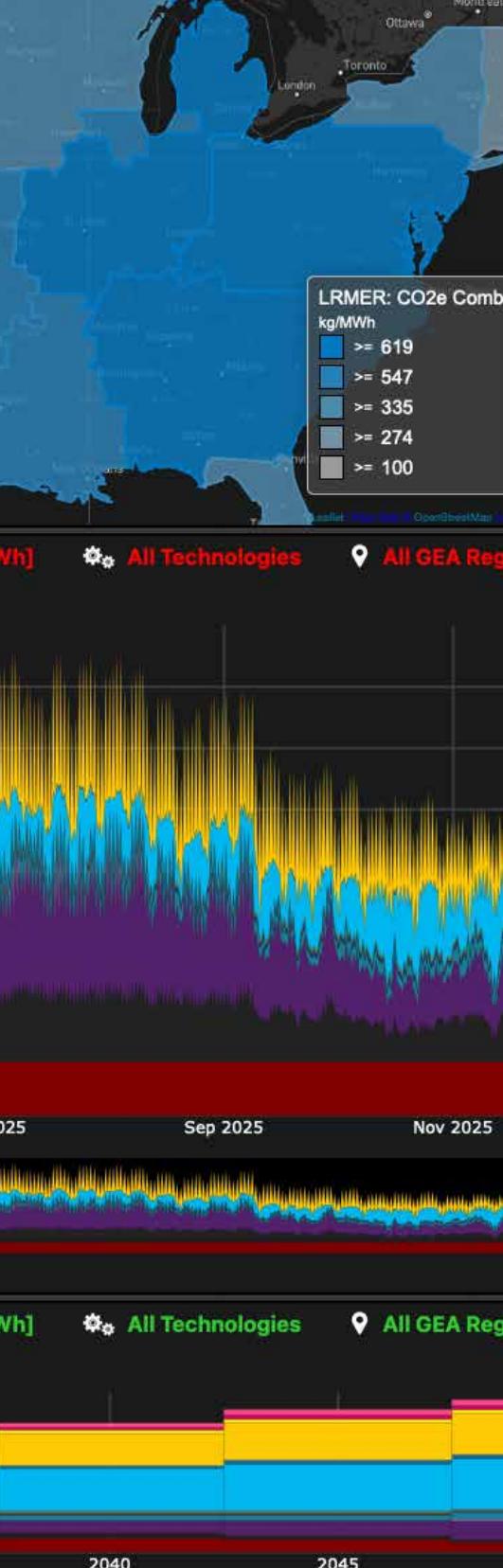
SolarAPP+ Facilitates Residential Solar Permitting and Installation

A 2024 R&D 100 finalist, the Solar Automated Permit Processing+ (SolarAPP+) web-based platform automates solar permitting for local governments and other authorities. Funded by the DOE Solar Energy Technologies Office, SolarAPP+ fosters rooftop solar adoption by making it easier for local governments to quickly and safely approve standardized rooftop projects. Since 2021, the collaborative effort has brought NREL, key code officials, and the solar industry together to develop standardized plan review software that can run compliance checks and process building permit approvals for eligible rooftop solar systems. SolarAPP+ helps jurisdictions review residential solar applications more easily by automatically checking system designs for safety and code compliance—and it helps installers by reducing install times, reducing project cancellations, and expanding access to energy by streamlining aspects of the permitting process. The R&D 100 has honored research and development in science and technology for over 60 years. SolarAPP+ was one of 141 finalists in 2024.

Cambium Datasets Help U.S. Electric Sector Decision Makers

In a rapidly changing sector, it is helpful if decisions about long-lived assets are supported by projections looking ahead over the coming years and decades. NREL's Cambium tool provides datasets of projected future values of the U.S. electric sector through 2050. The datasets are released annually and include simulated hourly emission, cost, and operational data for a range of modeled futures of the U.S. electric sector, with metrics designed to be useful for long-term decision-making. The data created in this project has been downloaded thousands of times for a variety of users, who use the data to inform their decisions and research. Cambium accompanies NREL's Standard Scenarios, which are an annually released set of projections of how the U.S. electric sector could evolve across a suite of different potential futures but covering more scenarios with less temporal granularity. The 2024 release—the fourth annual edition of Cambium—reflects changes in technology, market, and policy, as well as improvements to the underlying models.

# BRIDGING TO THE DEPARTMENT OF ENERGY LEADERSHIP COMPUTING

Computational scientists from across DOE advance energy innovation by leveraging the full DOE computing landscape.

Mistaken Identity: Mn_3AlN Is Actually Antiperovskite Mn_4N

Antiperovskites are inorganic compounds with unique structures that are of interest for their superconductivity and potential for use in energy storage. Mn_3AlN was first reported in 2011 as a perovskite and soft ferromagnet. With funding from the DOE Office of Science, researchers—intrigued by Mn_3AlN's classification as a soft ferromagnet—decided to investigate Mn_3AlN as it is the only example of a Mn_3AN compound with ferromagnetic behavior. Using Kestrel combined with compute resources at the National Energy Research Scientific Computing center, the team carefully investigated Mn_3AlN—attempting its synthesis and only developing antiperovskite Mn_4N or its precursors—and concluded, supported by DFT calculations, that it is more consistent with Mn_4N. Following the previously published synthesis method and exploring other reactions, they were unable to synthesize Mn_3AlN, leading them to the conclusion that Mn_4N was the compound erroneously identified as Mn_3AlN. This work clarifies that Mn_3AlN is not the only ferromagnetic Mn_3AN compound because it does not exist. Materials discovery is an important endeavor for expanding the opportunities of materials utilization, especially in emerging application areas that are based on novel phenomena, including magnetic and quantum behavior.

Unlocking Wind Farm Physics Across Vast Spatiotemporal Scales

Wind farm physics involve air-flow dynamics ranging from micron-thick boundary layers over blade surfaces to kilometer-wide atmospheric areas. Though high-fidelity models are computationally intensive and costly, they are currently the most promising method to accurately capture wind dynamics across these vast spatiotemporal scales. The biggest challenge with high-fidelity modeling is developing algorithms that capture complex wind phenomena and run efficiently on HPC systems. The DOE-funded ExaWind project, under the Exascale Computing Project, meets these challenges by offering powerful, GPU-enabled simulations that can accommodate high-fidelity models of wind farm physics. Leveraging DOE Wind Energy Technologies Office funds to use both Kestrel and Oak Ridge Leadership Computing Facility (OLCF) computational resources, NREL and Sandia National Laboratories researchers demonstrated and validated their high-fidelity models of turbulent air flow around turbines. On the OLCF Frontier supercomputer, researchers demonstrated the ability to simulate a wind farm composed of 16 5-MW turbines in a turbulent atmospheric boundary layer, using a model with about 38 billion grid points where resolution was sufficient to capture blade boundary layers. On the Kestrel supercomputer, researchers performed key validation studies of wind turbines in field and wind tunnel configurations that are critical to establishing ExaWind code credibility.
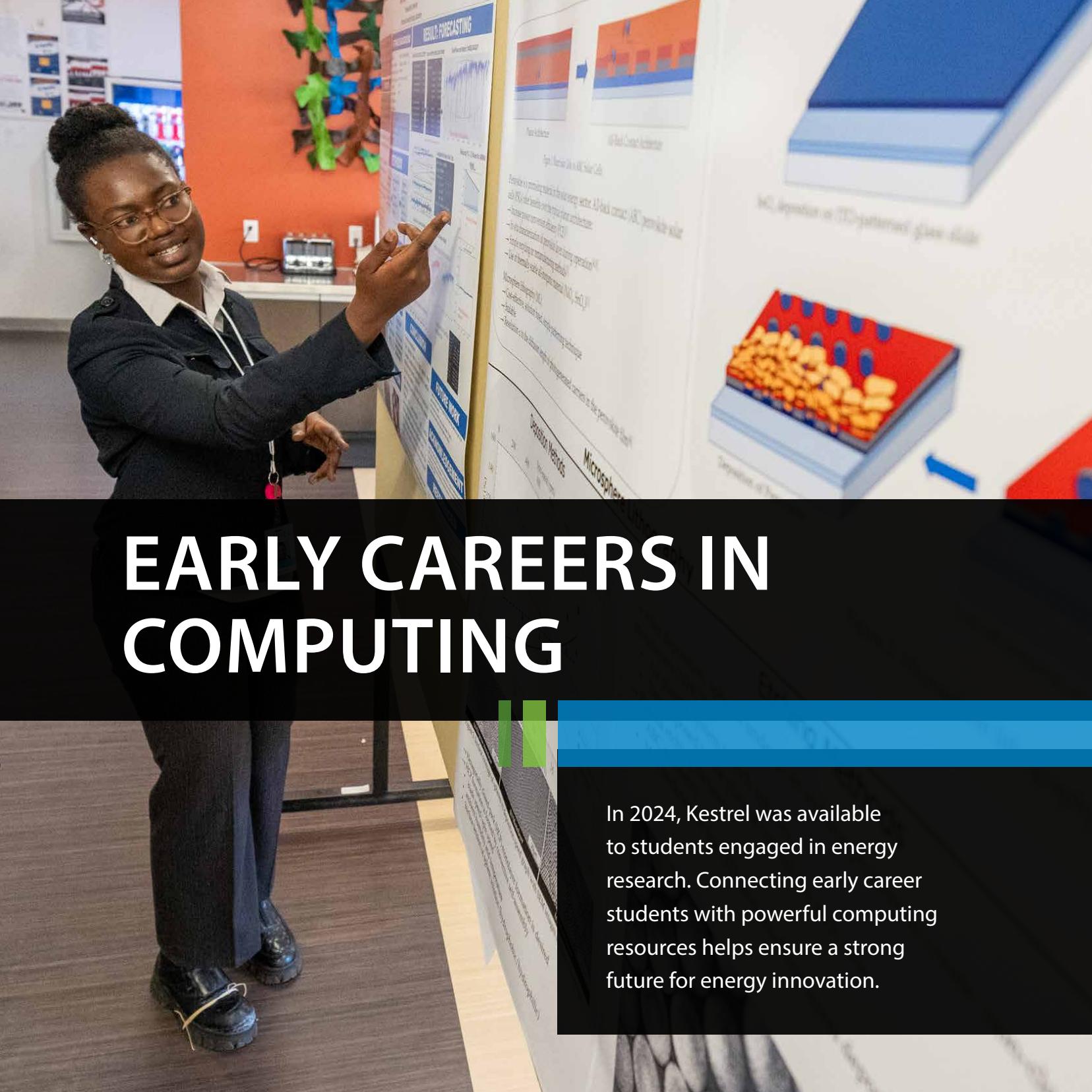
EARLY CAREERS IN COMPUTING

In 2024, Kestrel was available to students engaged in energy research. Connecting early career students with powerful computing resources helps ensure a strong future for energy innovation.

# Understanding Fuel Cell Device Complexity With AI

In collaboration with NREL researchers, graduate students from Rensselaer Polytechnic Institute and New Mexico State University used Kestrel to complete their dissertation work using AI to understand transport and reactivity in fuel cell devices, with funding from the DOE Hydrogen and Fuel Cell Technologies Office's ElectroCat Consortium. Electrocatalytic devices are well-known for their complexity, with catalysts, polymer electrolytes, ionic and gaseous species, and water all participating in key reactions and transport mechanisms that determine overall device performance. Describing these multicomponent devices accurately is beyond traditional classical and quantum mechanical simulation methods, so the research team developed an AI model of an important fuel cell catalyst: hydrated platinum with Nafion as the polymer electrolyte. Using state-of-the-art equivariant graph neural networks and leveraging Kestrel's powerful GPUs for both training of and prediction with the AI model, they constructed a realistic representation of this catalyst and studied transport properties near and far from the catalyst-polymer interface, as well as reactivity of important species such as oxygen. Such a combined model of transport and reactivity has been previously impossible due to limitations in accuracy (size) for classical (quantum) simulation methods. The ultimate goal of this work is to quickly develop AI models of electrocatalytic devices for any underlying chemistry, catalyst, and polymer electrolyte, allowing for rational understanding and design of complex devices across various economic sectors.

Building a Database To Train Neural Networks

Calculating drag is a core component of automotive exterior design as it affects energy loss significantly at high speed, affecting top speed, fuel efficiency, and stability. However, drag calculation is computationally expensive, requiring one CFD simulation per data point. Add in the complexity of modern vehicle design and the proprietary nature of commercial designs, and there are greater complications to calculating drag. Taking advantage of the new student allocation process on Kestrel, student researchers from Stanford University developed a method for generating datasets for predicting drag for automotive geometries, starting from a small number of beginning designs. They constructed a database of large eddy simulation flow fields used to train a convolutional neural network model for predicting aerodynamic performance. They tested the strategy using a realistic automotive geometry, with results showing that the convolutional neural networks predicted drag coefficients and surface pressures well. The researchers aim to complete the database with 10,000 samples, which would make it the largest openly available database of realistic automotive geometries.

Computational Model Depicts Hydrogen's Effect on Uranium Corrosion

Uranium is the primary fuel for nuclear applications but is also its primary waste product. Understanding uranium corrosion is critical for storing it at nuclear power plants. Preventing uranium corrosion will enhance safety and reduce the cost of storage at power plants. Student researchers from the University of California, Davis modeled and isolated hydrogen's interaction with defect sites in the oxidation layer to understand the corrosion process. They identified defects in the corrosion process using DFT and will validate their findings under experimental conditions, including room temperature and burnt fuel scenarios. Future work will focus on developing machine-learned force fields that provide similar accuracy as DFT but at 1,200 times lower computational cost.
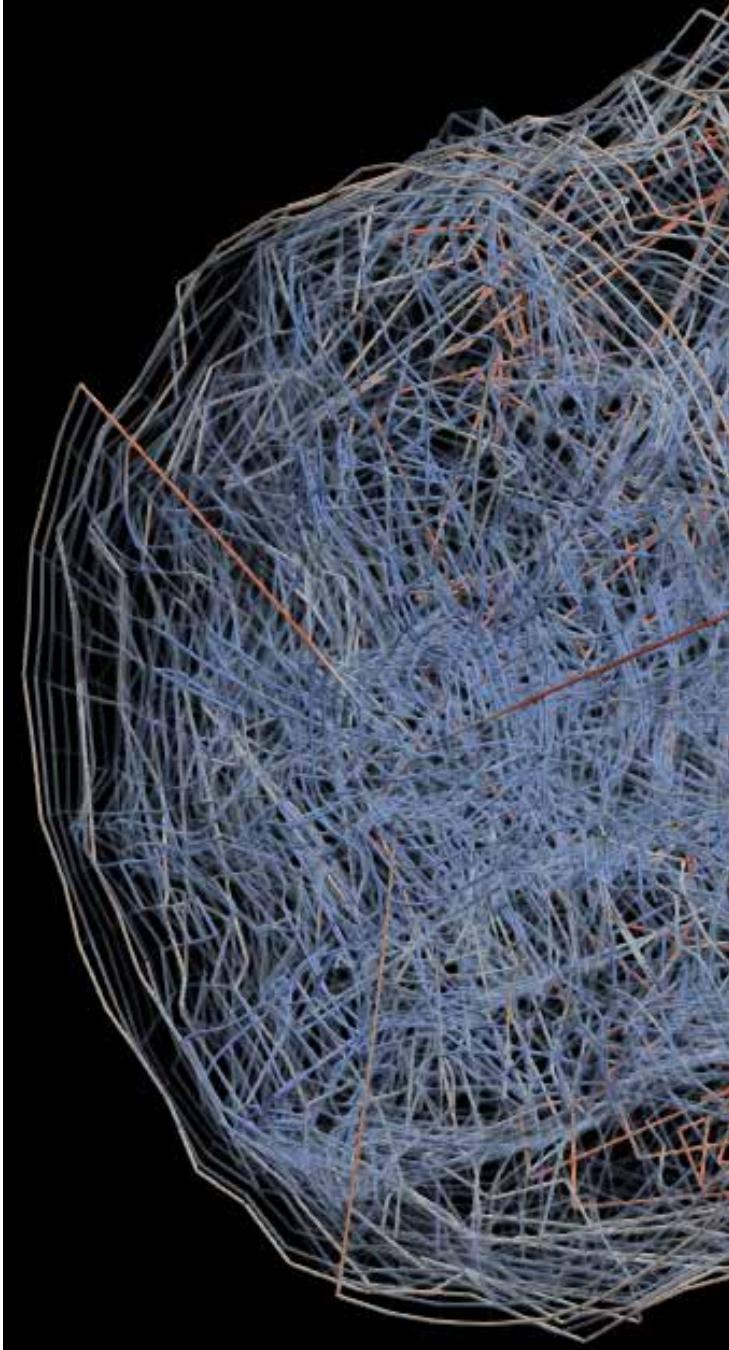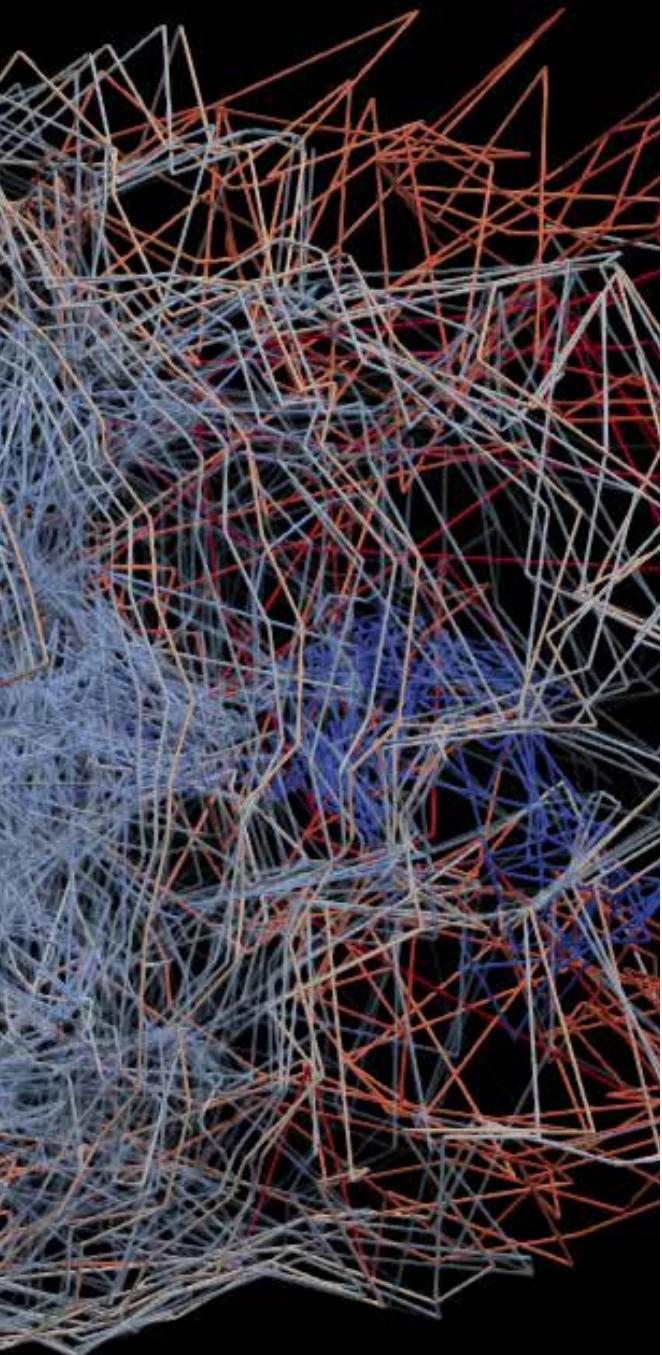
Low-Induction Rotor Design Could Reduce Wind Turbine Lifetime Fatigue and Improve Energy Capture

Current research trends in wind include more efficient and cost-effective wind plants, whether through novel turbine control strategies or new turbine technologies. As part of the Low-Induction Rotor Wakes project—a collaborative doctoral research effort between NREL and Penn State—performance of a novel wind turbine design for future wind plant applications was investigated. The design is known as a low-induction rotor: blade design is optimized to operate below traditional power production optimum to reduce lifetime fatigue loads but has an increased rotor diameter to improve energy capture per turbine.

The wind plant study was conducted using the NREL-developed Simulator for Wind Farm Applications (SOWFA), a high-fidelity computational fluid dynamics solver that couples realistic atmospheric boundary layer flows with wind turbine models for full wind plant simulation. Computationally expensive, high-fidelity wind plant simulations that are typically unfeasible at the university level were made accessible thanks to Kestrel. Metrics for assessment of the novel design include the velocity deficit and turbulence statistics in the wake, as well as total turbine power production and fatigue loads. The outcomes of the project will improve the broader scientific community's understanding of the low-induction rotor concept, as well as provide insight into how clever wind turbine design can improve overall wind plant performance.

INNOVATIONS AND PUBLICATIONS

Software Records

Title	NREL Number
AC (Adaptive Computing)	SWR-24-106
acopf_benchmarks (AC Optimal Power Flow Benchmarks)	SWR-24-43
AIM Benchmark (Application Benchmark for Quantum Computing Readiness in Clean Energy)	SWR-24-45
BBOpt (Black-Box Opt)	SWR-24-57
BiRD (BioReactorDesign)	SWR-24-35
BuildingsBench: A Benchmark for Universal Building Load Forecasting	SWR-23-51
CloudCV (Computer Vision on Edge Devices for the Short Term Prediction of Cloud Cover Supplementary Code)	SWR-24-119
EVI-Rental	SWR-24-74
Fair Bagging Boosting Models FKA: Fair Forest Models	SWR-24-38
FLCPVPanel (Fort Lewis College PV Panel Visualization Server)	SWR-24-117
FRISM (FReight Integrated Simulation Model)	SWR-24-40
HERO (Hybrid Environment Resources and Operations)	SWR-24-116
Maniac.jl (MANIfold optimization of AC power flow)	SWR-24-44
MLUQ (Uncertainty quantification for ML closure models)	SWR-24-36

Title	NREL Number
MODAQ (Modular Offshore Data Acquisition System)	SWR-24-58
MODAQ-BB (Modular Offshore Data Acquisition System - Blackbox)	SWR-24-72
MPI-Based Stochastic Programming in PYthon	SWR-24-113
N-S3 Cellular Vehicle-to-Everything (C-V2X) Cosimulation Framework	SWR-24-54
Primal-Dual Differentiable Programming for Critical Load Restoration Problems	SWR-24-41
PT-MELT (PyTorch Machine Learning Toolbox)	SWR-24-110
PVMesh	SWR-24-123
Red Teaming for Grid Cybersecurity	SWR-24-111
SPADES (Scalable Parallel Discrete Events Simulation)	SWR-23-99
SPADES (Scalable Parallel Discrete Events Simulation)	SWR-24-99
SysCaps (Language Interfaces for Simulation Surrogates of Complex Systems)	SWR-24-97
Udon (Unity Udon)	SWR-24-118
vidyut3d (Vidyut3d: a non-equilibrium plasma modeling tool)	SWR-24-101
WFM inference	SWR-24-139

Journal Articles

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3. Alberi, Kirstin, Chase Brooks, Ian Leahy, and Stephan Lany. 2024. "Tutorial: Defects in Topological Semimetals." Journal of Applied Physics 136 (9). https://doi.org/10.1063/5.0217533.

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6. Babinec, Susan, Ian Baring-Gould, Amy N. Bender, Nate Blair, Xiangkun Li, Ralph T. Muehleisen, Dan Olis, and Silvana Ovaitt. 2024. "Techno-Economic Analysis of Renewable Energy Generation at the South Pole." Renewable and Sustainable Energy Reviews 193 (April). https://doi.org/10.1016/j.rser.2023.114274.

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