



American Physical Society Global Summit 2026
Topical Group on Energy Research and Applications (GERA) Energy Workshop
Sunday, March 15, 2026
Convention Center, Mile High Ballroom
2A/3A
All Times Mountain Daylight Time (MDT)

- 8:30-8:40 Welcome Remarks from GERA Leadership
Billy Stanbery, GERA Chair
- Session 1:** Chair: Ramakrishna Podila, GERA Vice Chair
- 8:40-9:20 *MaterialEyes — Seeing the Invisible in Energy Materials using Experiment, Theory, and AI*
Maria Chan, Argonne National Laboratory (ANL)
- 9:20-10:00 *Modulating the Battery Performance Metrics by Tuning the Chemical Bonding in Oxide Cathodes*
Arumugam Manthiram, University of Texas at Austin
- 10:00-11:20 Coffee break and Poster Group 1
- Session 2:** Chair: Billy Stanbery, GERA Chair
- 11:20-12:00 *Time resolved optical spectroscopy of electrochemical dynamics at reactive surfaces*
Tanja Cuk, University of Colorado at Boulder
- 12:00-1:30 Lunch and Poster Group 2
- Session 3:** Chair: Tuan Anh Pham, Lawrence Livermore National Lab
- 1:20-2:00 *Metal Halide Perovskite Semiconductors for Photovoltaics and Beyond*
Joey Luther, National Laboratory of the Rockies, formerly the National Renewable Energy Laboratory
- 2:00-2:40 *AI-Driven Automated Experimental Platform for Accelerated Energy Materials Discovery*
Andy Huang, MTI Corporation
- 2:40-2:55 Break
- 2:55-4:15 Reception and Poster Group 3
- 4:15-4:30 Poster Award Ceremony: Rama Podila, GERA Vice-Chair

The 2026 GERA Energy Workshop is sponsored by the Topical Group for Energy Research and Applications (GERA) of the American Physical Society, the US Department of Energy, MTI corporation, AIP Publishing, and APS Publishing.

MaterialEyes — Seeing the Invisible in Energy Materials using Experiment, Theory, and AI

Maria Chan, Center for Nanoscale Materials, Argonne National Laboratory

In the development of materials for realistic applications, the detection and understanding of atomic and electronic structures, especially of defects, interfaces, and nanostructures, is paramount. Advances characterization via electron, x-ray, and atom probes, in imaging, scattering, and spectroscopic modes, have brought us closer to such detection and understanding. However, such experimental data is often difficult to parse and relate to fundamental understanding of mechanisms and behavior at the atomic level. In this talk, I will discuss our efforts in MaterialEyes to use AI/ML and theoretical modeling to enable the seeing of atomic structures from experimental characterization data. I will also discuss our work in using AI to extract and use microscopy and spectroscopy data from scientific literature, and in developing data standards for materials science. Examples will be drawn from a variety of energy materials, including batteries, catalysts, and photovoltaics. I will also discuss the Materials Acceleration Platform crosscut in the Energy Storage Hub Energy Storage Research Alliance (ESRA), a US Department of Energy Energy Innovation Hub.

Modulating the Battery Performance Metrics by Tuning the Chemical Bonding in Oxide Cathodes

Arumugam Manthiram, Walker Department of Mechanical Engineering, The University of Texas at Austin

In adopting a specific battery technology, six performance metrics need to be considered. They are cost, energy density, power density, cycle life, safety, and environmental impact. The six metrics are linked to severe materials challenges, and they need to be balanced, often with tradeoffs, depending on the specific application. 75% of the battery cost is due to materials, and about 50% of the materials cost is due to cathodes. Cathodes also limit energy density due to limited capacity and impact safety and cycle life. Among the various cathode chemistries explored over the years, both oxide and polyanion oxide cathodes are at the forefront for both lithium-ion and sodium-ion batteries. The performance metrics of oxide and polyanion oxide cathodes are linked to three fundamental factors: electronic configuration of metal ions, chemical bonding, and surface chemical reactivity with ambient air or electrolyte. Chemical bonding here refers specifically to the degree of covalence in the metal-oxygen bond, which is related to the charge transfer gap between metal: 3d and oxygen: 2p bands.

This presentation will focus on how the degree of covalence in the metal-oxygen bond sensitively influences cell voltage, capacity, electron and ion transport, rate capability, bond strength, thermal stability, gas evolution, safety, surface chemical reactivity, cycle life, etc. The sensitivity will be illustrated with specific examples of cathode compositions and electrolytes for both lithium-ion and sodium-ion batteries. The power of advanced characterization methodologies and electrochemical measurements in understanding the intricacies involved will be discussed. The fundamental understanding presented will help make advances in new materials design as well as in enhancing battery performance metrics, while keeping the \$/kWh affordable with acceptable cell safety.

Time-resolved Optical Spectroscopy of Electrochemical Dynamics at Reactive Surfaces

Tanja Cuk, Department of Chemistry, University of Colorado at Boulder

Catalytic reaction pathways on surfaces have long been a target of experimental physical chemistry in a variety of environments. A recent pursuit has been the detection of molecular intermediates buried within the electrode-electrolyte interface of energy storage technologies. Coincident with this detection is isolating the intermediates in time and following their electrochemical dynamics, as one intermediate leads to another in multi-step reactions. Time resolved optical spectroscopy from femto- to micro- seconds follows the highly efficient, photo-driven oxygen evolution reaction from water at titanium oxide surfaces. This talk will explain how the experimental setup is conducive to the goal and summarize the accomplishments across the visible and infrared probes. The excited state spectra are assigned to adsorbed oxygen intermediates by agreement with theoretical predictions of titanium-oxide distortions around trapped holes or hole-polarons. The dynamics of the excited state spectra resemble that of a catalytic pathway, with ultrafast formation of intermediates, a long range of nanosecond meta-stability, and finally their decay at microsecond

timescales. The populations and their dynamics are strongly influenced by the electrolyte conditions, with pH controlling the protonation of the reactive oxygen. Open questions remain of how to understand the concerted dynamics of the excited state visible absorptions, visible emissions, and infrared vibrations for a more complete description of the catalytic pathway.

Metal Halide Perovskite Semiconductors for Photovoltaics and Beyond

Joseph M. Luther, Senior Research Fellow, National Lab of the Rockies (previously known as NREL)

The overall photovoltaics industry is growing rapidly and may move toward new semiconductor technologies and new approaches to generate and use that electricity. In 2020, a terawatt (TW) of total installed capacity was surpassed, and now the 2nd TW of installed capacity was recently surpassed. PV markets are also expanding now as well with many applications from residential, to utility scale (embedded in agriculture, or on water), and satellites in space and more.

This presentation will highlight key history and showcase new PV technologies, involving semiconductors such as perovskites which provide a potential leap forward in terms of higher efficiency and lower cost products. Perovskites also have a growing domestic industry and are now reaching commercialization. But photovoltaics are not the only promising avenue for this evolving material platform. There are a variety of applications well beyond PV where perovskites could be exploited for their fascinating properties. I will show a variety of novel spin-based applications where chirality can be imparted leading to new levels of control.

AI-Driven Automated Experimental Platform for Accelerated Energy Materials Discovery

Andy Huang, MTI Corporation, CA, USA

The development of advanced functional materials—particularly for energy storage, catalysis, and electronic applications—is often hindered by slow, manual, trial-and-error experimental workflows. As the demand for rapid innovation in material science grows, there is a critical need for self-driven laboratory (SDL) systems that couple artificial intelligence (AI) with highly automated hardware infrastructure. These systems promise to significantly reduce the discovery time of novel materials by integrating closed-loop feedback, autonomous decision-making, and precision-controlled experimentation. This work introduces a fully integrated, AI-driven automated experimental platform designed to support self-driven materials research. The platform emphasizes reliable high-throughput synthesis, robust characterization, and adaptive decision-making through automated equipment that ensures precision, repeatability, and scalability.