

U.S. DRIVE Highlights of Technical Accomplishments

2023





U.S. DRIVE Highlights of Technical Accomplishments Overview

Through precompetitive collaboration and technical exchange, U.S. DRIVE accelerates the development of energy-efficient advanced automotive and energy infrastructure technologies.

U.S. DRIVE (*Driving Research for Vehicle efficiency and Energy sustainability*) is a voluntary governmentindustry partnership focused on precompetitive, advanced automotive and related infrastructure technology research and development. Partners are the United States Department of Energy (DOE) and leaders in the automotive industry (United States Council for Automotive Research LLC, the collaborative technology company of Ford Motor Company, General Motors, and Stellantis); energy industry (BP, Chevron, Phillips 66, ExxonMobil, and Shell); and electric utility industry (American Electric Power, DTE Energy, Duke Energy, Southern California Edison, and the Electric Power Research Institute).

The Partnership benefits from a history of successful collaboration across multiple technical areas, each focused on a key area of the U.S. DRIVE portfolio (see below). These teams convene the best and brightest scientists and engineers from across the Partnership to discuss key technical challenges, identify possible solutions, and evaluate progress toward goals and targets published in technology roadmaps. By providing a framework for frequent and regular interaction among technical experts in common areas of expertise, U.S. DRIVE accelerates technical progress, helps to avoid duplication of efforts, ensures that publicly funded research delivers high-value results, and overcomes high-risk barriers to technology commercialization.

U.S. DRIVE teams selected the highlights in this document from many hundreds of DOE-funded projects conducted by some of the nation's top research organizations. Each one-page summary represents what Partnership experts collectively consider to be significant progress in the development of advanced automotive and infrastructure technologies. The report features technical highlights in two general categories:

Vehicles

- Electric Drive
- Electrochemical Energy Storage
- Fuel Cells
- Materials
- Vehicle and Mobility Systems Analysis

Infrastructure and Integration

• Grid Integration

More information about U.S. DRIVE, including prior-year accomplishments reports and technology roadmaps, is available on the DOE (<u>https://www.energy.gov/eere/vehicles/us-drive</u>) and USCAR (<u>www.uscar.org</u>) web sites.

Contents

VEHICLES	1
Electric Drive	1
Development of Sustainable High-Performance Magnets for Exceptional Power Density Electric Drive	ີ ວ
Niolois	. Z
Medified DBC Substrate for Space Destricted Application	. 3
Motor with Advanced Cancents for High newer density and INtegrated cooling for Efficiency (MACHINE)	.4
Fabrication of Soft Magnetic Components with High Volume Loading of Fe ₄ N	. 6
Electrochemical Energy Storage	7
Development of New High-Energy Cathodes Containing 60% Manganese	. 8
Stabilizing Cobalt-Free Cathodes with Lithium Stoichiometry Control	. 9
An Inorganic-Rich Interphase for Lithium Metal Batteries with Improved Cycle Life	10
Room Temperature Rechargeable Solid-State Lithium-Air Battery	11
Binder Design for Recyclable Batteries	12
Enhanced Energy and Improved Cyclability of Earth-Abundant Cathodes	13
Investigating High-Voltage Lithium Cathode-Electrolyte Interfaces	14
Fast Diagnosis of Li-ion Battery Health from High-Rate Data using Artificial Intelligence	15
Silicon Anode Technology for Next-Generation Lithium-Ion Batteries	16
Carbon Coatings Improve the Cycling Performance of Disordered Rocksalt Cathodes	17
Advancing All-Solid-State Lithium-Sulfur Battery through Materials and Interfacial Innovations	18
Enabling Fast-Charging in Solid-State Batteries	19
Transport-Regulating Polymer Coating to Improve the Cyclability of Lithium-Metal Batteries	20
High-Entropy Electrolytes for Lithium-Metal Batteries	21
Fuel Cells	22
Reducing the Cost of Compressed Hydrogen Storage	23
Reducing the Cost of Owning Hydrogen Fueled Vehicles	24
Materials	25
Manufacturing Demonstration of a Large-scale, Multi-Material Passenger Vehicle Sub-system	26
Modeling Damage Accumulation in Corrosion of Polymeric Adhesives	27
Changing the Design Rules of Rubber to Create Better Wearing, Lighter Weight, More Fuel-Efficient Tires	; 28
Bio-based, Inherently Recyclable Epoxy Resins to Enable Facile Carbon-Fiber Reinforced Composites	20
A Novel Manufacturing Process of Lightweight Automative Secto	29
A Novel Manufacturing Process of Lightweight Automotive Seats	21
High Velocity (HiVe) Joining: Encluing Multi Meterial Jointe	21
High Velocity (HIVE) Johning. Eliability Matrix Compositos for Higher Efficiency EV Dewertreine	32 22
Meeting Learning for Automated Weld Quality Manitaring and Control	33 24
Solid Phase Processing of Aluminum Castings	35
Vehicle and Mobility System Analysis	36
Vehicle Automation Impact on Mobility and Energy	37
INFRASTRUCTURE AND INTEGRATION	38

Grid Integration	38
Cerberus: A Cyber-physical Security Mitigation Solution for High-Power EV Charging Infrastructure	39
Roadmap of Standards and Codes for Electric Vehicles at Scale (EVs@Scale)	40
Next-Gen Profiles Project	41

VEHICLES

Electric Drive



2023 U.S. DRIVE Highlight Development of Sustainable High-Performance Magnets for Exceptional Power Density Electric Drive Motors

Grain boundary engineering to replace heavy rare earth elements.

Ames National Laboratory

Ames National Laboratory (AMES) researchers have developed a grain boundary additive to improve the magnetic performance of fine-grained neodymium (Nd)-based sintered magnets. Minimizing the loss in coercivity at elevated temperatures in traction motors typically requires the addition of heavy rareearths (HREs). AMES has been developing processing methods to produce fine grain feed stock powders and their handling without HREs (e.g., dysprosium). An additional challenge when sintering ultrafine grain powders is to get a fully dense magnet without growing the grains since very high temperatures are required. The sintering temperature can be lowered if a suitable sintering aid can be added. However, these sintering aids must be tailored to the overall chemistry of the alloy since they must not degrade the magnetic properties of the matrix phase nor take up too much volume and dilute the effective work the magnet performs in a motor.



Figure 1. Demagnetization loops for samples without any sintering aids and their performance with increasing weight percent of the Pr-Al-Cu compound at room temperature.

Ames researchers tested two promising compounds, praseodymium (Pr)-copper (Cu) and Pr-Cualuminum (Al), both with melting points more than 250°C lower than the lowest peritectic reaction temperature in Nd-iron-boron alloy compositions used in typical traction motors. As shown in Figure 1, the sintering aid increases coercivity and slightly decreases remanence.

More importantly is how the grain boundary phase also affects the higher temperature performance of the magnet. Note (Figure 2), the magnet with 3 wt.% of sintering aid has the best performance.



Figure 2. Summary of temperature effect on energy product as a function of wt.% addition of Pr-Al-Cu.

Compared to a commercial alloy with 4.5wt.%Dy, the AMES alloy is only slightly lower in coercivity and has very similar thermal coefficients for remanence and coercivity as the commercial alloy.

Sample ID	no PrAlCu	3 wt% PrAlCu	7.5 wt% PrAlCu	Arnold N45H
Dy wt%	0	0	0	4
Br (kGs)	13.8	13.4	12.1	13.5
Hc (kOe)	13.5	15.6	17.6	17
(BH) _{max} (MGOe)	44.1	40.7	35.7	44
-α _{25-125°C} , %/°C	0.12	0.12	0.14	0.12
-β _{25-125°C} , %/°C	0.7	0.64	0.64	0.61

Table. 1. Comparison of magnetic properties.

Page 2 | Electric Drive Technical Team



2023 U.S. DRIVE Highlight Dielectric Fluid (Liquid) Cooling Demonstration Using a Silicon Carbide Module

Demonstrated reduced thermal resistance (20%) and pumping power (80%) using a dielectric fluid cooling solution.

National Renewable Energy Laboratory

The National Renewable Energy Laboratory (NREL) designed a new, dielectric fluid (liquid) cooling concept for power electronics. The concept uses dielectric fluids simplify to the package configuration and eliminate the thermally resistive ceramic component used in metalized ceramic substrates. The new concept incorporates dielectric fluid jets impinging on finned copper heat spreaders to cool silicon carbide (SiC) devices. Using dielectric fluids enables reduced junction-to-fluid thermal resistance by eliminating the ceramic component, allows for cooling other inverter components (e.g., capacitors, bus bars), and enables integrating the power electronics with the electric motor.

A thermal demonstration module was fabricated using two 650 volt (V) SiC metal-oxidesemiconductor field-effect transistor (MOSFET) devices. The two devices were connected in parallel and represented one electrical switch. The SiC devices were soldered to copper heat spreader substrates and installed within the dielectric fluid heat exchanger (Figure 1). The heat exchanger was made from polyphenylene sulfide and polyetheretherketone materials, which are hightemperature plastics, compatible with dielectric fluids, used in automotive applications, and are lightweight.

The assembled module and heat exchanger were piped into the dielectric fluid loop to circulate AmpCool-110 dielectric fluid. AmpCool-110 (from Engineered Fluids) is designed to cool the battery packs and electric machines in electric vehicles (EV), and hence is an appropriate fluid for this application. We are also collaborating with Infineum fluids to evaluate new driveline fluids that are being developed specifically for EVs.

The experimentally measured results show that the dielectric fluid concept can outperform water-

ethylene glycol (WEG) cooling systems (Figure 2). The dielectric fluid concept was found to reduce the junction-to-fluid thermal resistance and pumping power by 20% and 80%, respectively, compared to a WEG-cooled CREE SiC module. Additionally, the model predictions were found to be in good agreement with experimentally measured values.

A preliminary analysis was conducted to size an aircooled heat rejection system for the dielectric fluid which indicates that a 218-cm² folded-fin heat exchanger is required to dissipate 2.5 kW of heat assuming 50°C air temperature. This is about 8% smaller than a WEG-based heat exchanger. The size decrease is enabled by the dielectric's fluid's higher temperature compared with WEG. Long-term reliability for this flow configuration will also be investigated in the near future.



Figure 1. Pictures of the SiC module installed within the dielectric-fluid-based plastic heat exchanger (left). Modeling results showing the slot jet cooling design (right).





Modified DBC Substrate for Space Restricted Application

Designed and evaluated low thermal resistance modified DBC substrate

Oak Ridge National Laboratory

The traditional direct bonded copper (DBC) substrates do not utilize heat spreading because of the thinner copper layer, thus using a much smaller active surface area for cooling. To improve heat transfer, a modified DBC substrate has been proposed, named DBCwCu. The modification includes a thick copper block/tile in between the semiconductor device and the DBC substrate. This simple modification improves heat spreading underneath the die, thus using a much larger substrate area for heat transfer. Traditional and modified DBC substrates are shown in Fig. 1.

The modified DBC substrate's performance has been experimentally evaluated and compared with a traditional DBC substrate. Two half-bridge modules were made: one traditional DBC (Fig. 1, left) and one DBCwCu (Fig. 1, right) for comparison. A single Wolfspeed MOSFET was soldered in each switching position and was wire bonded to the substrate for gate, drain, and source terminations. The substrate was then attached to a heat sink using a thermal interface material and was clamped using a 3Dprinted structure. Two holes were made in the heat sink to place thermocouples underneath the substrate to capture the substrate's bottom surface temperature. The device surface was painted with matte black paint to increase emissivity, and the device temperature was captured using a thermal camera. Fig. 2 shows the thermal evaluation experimental setup. In this experiment, MOSFET body diodes were conducted to generate losses. A DC source was used to inject current through body diodes, and the top and bottom diodes were connected in series.

Fig. 3 plots the device temperature and thermal resistance improvement results. The traditional DBC substrate temperature reaches 160°C with 180W Power Loss whereas the DBCwCu device temperature reaches the

same value when the injected loss was 250W. Results (Fig. 3, top) show that the modified DBCwCu substrate can handle 30% higher losses than the traditional DBC, which implies the improved thermal resistance shown in Fig. 3.



Figure 1. Assembled substrate for thermal evaluation: the conventional direct bonded copper (DBC) substrate (left) and the modified DBC with copper substrate (right).



Figure 2. Experimental setup to evaluate the thermal performance of the proposed DBC with copper substrate.





2023 U.S. DRIVE Highlight Motor with Advanced Concepts for High power density and INtegrated cooling for Efficiency (MACHINE)

In-slot embedded cooling reduces winding temperature by 50% by reducing thermal resistance from source to sink by 65%.

RTX Technology Research Center (RTRC)

Electric motor power density and efficiency are limited by design trade-offs between material options, electromagnetics, thermal management, and structural design considerations. The RTRC team has developed a Motor with Advanced Concepts for High power density and INtegrated cooling for Efficiency (MACHINE), demonstrating an 8X improvement in power density by leveraging three key technology elements: (a) use of non-heavy rare earth hard magnets, (b) high silicon soft magnetic steel, and (c) embedded in-slot cooling (Figure 1). To achieve better performance, the team utilized multi-physics design optimization methods to maximize the optimal magnetic loading, electric loading, and airgap shear stress while efficiently removing the generated heat.



Figure 1. Developed MACHINE concept with embedded cooling channels and non-heavy rare earth magnets.

The developed MACHINE concept considers surface permanent magnet rotor architecture with fractional slot concentrated windings along with embedded inslot cooling. With optimization, it is designed to handle ~17-20 Arms/mm² for a select duty cycle. The team has developed a multi-physics analysis and design framework as shown in Figure 2 to verify the design operation and performance including electromagnetics, thermal, structural and flow distribution into the cooling channels. The motor winding design was optimized for overall performance while considering manufacturability.



Figure 2. Multi-physics design optimization of MACHINE concept.

The RTRC team has successfully completed building, testing and validation of a sectional stator with embedded cooling channels with ethylene glycol water (EGW) 50:50 coolant. The team then compared experimental results with high fidelity model predictions, and updated finite element models to reflect experimental conditions. A series of experimental tests and model analysis at various conditions are shown in Figure 3. The model predicted temperature matches well with the experimental temperature measurements.



Page 5 | Electric Drive Technical Team



2023 U.S. DRIVE Highlight Fabrication of Soft Magnetic Components with High Volume Loading of Fe₄N

Earth-abundant soft magnetic composites for electric machines and power electronics.

Sandia National Laboratories

Sandia National Laboratories has developed highmagnetization, low-loss, earth-abundant, ironnitride-based (Fe₄N) soft magnetic composites (SMCs) and has successfully formed them into components for electric machines and motor drives. These new magnetic components will enable low eddy current losses and highly efficient motor operation at rotational speeds up to 20,000 rpm at temperatures up to 150°C. As our capability to produce Fe₄N/epoxy samples has improved, we have progressed to the fabrication of larger parts, which is key to the utilization of these materials in automotive systems.

This year, our team devoted significant effort to the fabrication of soft magnetic parts for a dual rotor homopolar AC machine (DHAM) designed by our collaborators at Purdue University. A benefit to fabricating soft magnetic motor parts using SMCs is that a monolithic Fe_4N composite can replace a stack of many electrical steel laminations, and moreover this machine design does not require permanent magnets. The first parts fabricated used a molding process, where computer-aided design drawings of the soft magnetic parts were shared by Purdue and were used to 3D print anti-molds at Sandia using polylactic acid. Using this method, a 50% scaled version of the short stator assembly was fabricated using 55 vol.% Fe_4N in epoxy (Figure 1).



Researchers evaluated a die for a DHAM rotor in Sandia's current hot pressing setup. This die is significantly larger than any others used previously in our lab, so a new heating band and approach to heating was required. The temperature of the die was closely monitored at several physical points until a method for consistent heating was established. Once the uncured composite is in the die, the preheated anvil is inserted and the composite is pressed at 37 MPa. This is significantly lower than the pressure used for smaller pressed parts due to the size and shape of the DHAM rotor assembly and die.



Figure 2. DHAM rotor assembly during removal from custom hot pressing die.

Carbon paper was utilized between the base and the outer die to ensure that the base and sample could be demolded. This worked well, and the demolding process was performed effectively. Currently, samples have been demolded with very few or negligible defects such as hairline fractures or chipping along the inner or outer edges (Figure 2). Components such as this will greatly facilitate rareearth-free motor components that can be readily fabricated, as well as magnetic components (e.g. inductor cores) for motor drives.

Electrochemical Energy Storage

2023 U.S. DRIVE Highlight

Development of New High-Energy Cathodes Containing 60% Manganese

Novel, Mn-rich cathode developments reveal effective new strategies for enabling future sustainable cathode-materials.

Argonne National Laboratory

In our fiscal year 2021 highlight, the Materials Research Group at Argonne National Laboratory reported the development of novel cobalt (Co)-free Li₂MnNiO₄ cathodes based on lithiated-spinel structures. [Chem. Comm. (2021),doi.org/10.1039/D1CC04334J]. These lithiumexcess spinels (LxS) surpass conventional spinels such as LiMn₂O₄ and LiMn_{1.5}Ni_{0.5}O₄ by doubling the lithium (Li) concentration in their pristine states, while maintaining cubic symmetry. Li//LxS-L₂MnNiO₄ cells exhibit remarkable energy densities, delivering ~225 mAh/g capacity between 2.5 - 5.0 volt (V) (similar to or exceeding state of the art cathodes), with nearly 96% retention after 50 cycles (Figure 1 (c)). The exceptional electrochemical performance of high-Mn LxS is attributed to the stable spinel framework and the inherent three-dimensional Li-ion diffusion pathways, facilitating rapid Li-ion diffusion. Our recent investigations have revealed a continuous topotactic phase transformation occurring between LxS and layered structures when the synthesis conditions are carefully controlled, suggesting the potential for precise modulation of the local atomic structural arrangements and associated electrochemical properties.

Increasing the manganese (Mn) content is a promising approach for sustainability of the Li-ion battery supply chain. A newly developed series of Mn-rich LxS cathodes, referred to as LxS-Li₂Mn_{1+x}Ni_{1-x}O₄ (0<x<0.5), exhibits an impressive specific capacity of up to 250 mAh/g when cycled between 2-5.0V vs. Li. Figure 1(a) shows a representative X-ray diffraction pattern of Li₂Mn_{1.2}Ni_{0.8}O₄ with the previously reported LxS-Li₂MnNiO₄. The refinement analysis indicates a significantly lower disordering ratio for LxS-

Li₂Mn_{1.2}Ni_{0.8}O₄ (11%) compared to LxS-Li₂MnNiO₄ (18%), suggesting a more ordered structure with increased Mn content. Consequently, the initial discharge capacity of LxS-Li₂Mn_{1,2}Ni_{0,8}O₄ improved from 225 to 250 mAh/g, increasing the energy density from 800 to 920 Wh/kg, while maintaining similar cycling performance as the LxS-Li₂MnNiO₄ (Figures 1(b) and (c)). Also, LxS-Li₂Mn_{1.2}Ni_{0.8}O₄ exhibits enhanced rate performance (Figure 1(d)), attributed to its more well-established three-dimensional Li-ion diffusion channels. The successful synthesis of high-performance Mn-rich LxS-LMNO not only broadens the compositional space of LxS materials but also positions them as promising, high-energy density and cost-effective next generation earth abundant cathode materials. These materials do not suffer from the widely known voltage fade phenomena of Li-Mn rich cathode, but future work may include the investigation of novel electrolyte formulations for high voltage operation.



performance, and (d) rate capability.

Page 8 | Electrochemical Energy Storage Technical Team

2023 U.S. DRIVE Highlight Stabilizing Cobalt-Free Cathodes with Lithium Stoichiometry Control

Developed a Li-stoichiometry control approach for synthesizing cobalt-free cathodes with a stabilized composite structure, aiming to improve long-life, sustainable batteries for powering electric vehicles.

Argonne National Laboratory, Brookhaven National Laboratory

Lithium-ion batteries (LIBs) play a crucial role in decarbonizing transportation. However, their heavy reliance on high-cost and scarce cobalt in many of their cathodes raises supply-chain and sustainability concerns. Eliminating cobalt (Co) from cathodes, while maintaining high energy, remains elusive, as doing so detrimentally affects their layering and cycling stability. Researchers from the Argonne and Brookhaven National Laboratories (ANL, BNL) designed a lithium (Li)stoichiometry control approach to synthesize Cocathodes, specifically LixNio.95Mno.05O2 free (NM9505). Structural and morphological control was achieved by tuning Li stoichiometry, resulting in a transition from large-sized particles (100s of nm) with a single layered phase to small layeredrocksalt composites (10s of nm) with decreasing Li Content (Figure 1).

Experimental characterization with computational modeling of the calcination process revealed the crucial role of Li stoichiometry in controlling the rocksalt-to-lavered phase transformation and crystal growth (Figure 2 (a)). These insights were used to synthesize Li-deficient compositestructured NM9505. This material does not require surface washing to remove lithium residue, promising potentially lower cost. Due to its low anisotropic lattice expansion and contraction during cycling, Li-deficient NM9505 exhibited 90% capacity retention and *close-to-zero* voltage fade (a common issue with Li and manganese [Mn] excess cathodes) for 100 deep cycles, showing its potential as a Co-free cathode for long-life, sustainable LIBs (Figure 2 (bc)).

ANL and BNL continue to explore this stoichiometry control approach to synthesize

various composite-structured cathodes for Li-ion, sodium (Na)-ion, and solid-state batteries.



Figure 2. (a) Particle size variation of the NM9505 as a function of Li over transition metal ratio, Li/TM. Inset: simulated particle microstructure for Li/TM= 0.95 and 1.05. Scale bars: 100 nm. (b, c) Capacity retention and voltage profiles of NM9505 with 0.95Li (red) and 1.05Li (black).

Page 9 | Electrochemical Energy Storage Technical Team



2023 U.S. DRIVE Highlight An Inorganic-Rich Interphase for Lithium Metal Batteries with Improved Cycle Life

*CsNO*³ was identified as a dual-functional additive to form good interphases on both NMC cathode and lithium metal anode to enable a lithium metal battery with long cycle life and fast charge capability

Brookhaven National Laboratory

Researchers identified CsNO₃ as a dual-functional additive to form good interphases on both the NMC cathode and lithium(Li) metal anode to enable a lithium metal battery (LMB) with long cycle life and faster charge capability. Using 1,2-dimethoxyethane (DME)-LiFSI based electrolyte containing the CsNO₃ additive, the LiNi_{0.8}Mn_{0.1}Co_{0.1}O₂||Li cell was cycled at a 1C rate and retained more than 80% of initial capacity after 200 cycles, even with a high cathode loading of 5mAh/cm² (relevant to EV batteries) and a low N/P ratio of 2. In contrast, the cell using the baseline electrolyte experienced a quick loss of capacity within 20 cycles, duplicate cells displayed similar behavior. The resulting interphase is anion-derived and dominated by the inorganic species CsFSI. It is free of LiF, which is the component commonly believed to be necessary for a good interphase. These results emphasize that the role of LiF in the solid-electrolyte interphase (SEI) may need to be reconsidered and the role of Cs⁺ in LMB electrolyte needs to be revisited.

The team constructed cells with a Li metal anode and an NMC811 cathode to compare the performance using the baseline electrolyte and that with CsNO₃ additive. Coulombic efficiency (CE) of the cell with the C_{sNO_3} additive is higher (99.46%) than the cell using the baseline electrolyte (99.11%). Using the baseline electrolyte, cells under mild conditions (250 µm thick Li, 9mg/cm² cathode) can maintain stable cycling for up to 70 cycles (Figure 1a). However, a rapid capacity drop is observed afterwards. In contrast, the electrolyte containing the CsNO₃ additive improved the cyclability of the cell under same conditions. Over 70% capacity retention is maintained even after 300 cycles (Figure 1a). The dramatic effect of using the CsNO₃ additive on fast charging was also observed. LMB cells first went through two formation cycles at C/10 rate and 5 cycles at C/5 rate and then were cycled at 1C rate. Even under harsh conditions (50 μ m thick Li foil, 21 mg/cm², NMC811 cathode, N/P ratio = 2), cells using electrolytes with the CsNO₃ additive maintain more than 80% of the initial capacity even after 200 cycles while the cell using the baseline electrolyte quickly loses its capacity within 20 cycles. These results indicate that both cathode and anode must have been well protected during the cycling, validating the dual protection strategy proposed.



in Figure 1a.

2023 U.S. DRIVE Highlight

Room Temperature Rechargeable Solid-State Lithium-Air Battery

A Li-air battery has been developed that demonstrates a very high energy density by using a solid-state electrolyte to enable a reversible four-electron reaction between lithium and oxygen.

Illinois Institute of Technology, and Argonne National Laboratory

There is a growing interest in developing new battery chemistries to replace current lithium (Li)-ion batteries that are based on Li intercalation into a metal oxide structure. One area of research has been Li-oxygen (Li-O₂) batteries based on the formation and decomposition of lithium peroxide (Li₂O₂). This product results from the two-electron reaction between Li⁺ and O₂ by either of the two pathways shown in Figure 1. This chemistry potentially has a much higher energy density than Li intercalation because of the formation of Li-oxygen bonds. The successful development of a battery based on Li₂O₂ chemistry could theoretically have several times the energy density of currently used Li-ion cells.

A Li-O₂ battery cell based on lithium oxide (Li₂O) formation and decomposition potentially has an even higher energy density than one based on Li₂O₂. This is because it is based on a four-electron reaction as shown in Figure 1, which does not stop at Li₂O₂ formation. The four-electron reaction can deliver an energy density about four times that of a Li-ion battery and thus will enable EVs with much longer range which is highly desirable. However, the four-electron reaction is much more difficult to achieve than the two-electron reaction that produces Li₂O₂.

Most Li-O₂ batteries use a liquid electrolyte for transport of Li cations between the anode and cathode where the Li_2O_2 product is formed. However, research teams from the Illinois Institute of Technology and Argonne National Laboratory have found that by using a solid-state electrolyte in a Li-O₂ battery the product formed on the cathode is Li₂O and not Li₂O₂. The solid-state electrolyte used is a composite polymer electrolyte fabricated from Li₁₀GeP₂S₁₂ nanoparticles embedded in a modified polyethylene oxide polymer matrix. In lab testing of a coin cell, the battery is rechargeable at 1000mAh/g capacity for 1,000 cycles at a 1C rate with a low polarization gap at room temperature, as shown in Figure 2. The battery can run in an air atmosphere and is thus referred to as Li-air battery. A new chemistry based on fast transport of Li cations through the solid-state electrolyte is believed to enable the reaction (Scheme I in Figure 1) to reach the four-electron product, Li_2O , and not stop at Li_2O_2 .

Further work is planned to investigate large cell performance.

$$O_{2}^{*} \xrightarrow{e^{-}} O_{2}^{-*} \xrightarrow{Li^{+}} LiO_{2}^{*} \xrightarrow{e^{-}, Li^{+}} Li_{2}O_{2}^{*} \xrightarrow{2e^{-}, 2Li^{+}} 2Li_{2}O^{*}$$
(I)

$$LiO_{2}^{*} \xrightarrow{(E)} G_{3}$$

$$Li_{2}O_{2}^{*}, O_{2}$$

$$Li_{2}O_{2}^{*} \xrightarrow{(F)} Li_{2}O^{*}, O_{2}$$
(II)

Figure 1. Two possible reaction pathways to the formation of Li_2O from reaction of O_2 , Li^+ , and e^- . The reaction highlighted by yellow is the one occurring in the solid-state Li-air battery.



Figure 2. Solid-state Li-air battery cell performance at a limited capacity of 1000 mAh/g showing galvanostatic cycling over 1000 cycles and a small polarization gap.

2023 U.S. DRIVE Highlight Binder Design for Recyclable Batteries

An electrode binder can quickly release the different components of battery electrodes into their individual forms for low-cost, convenient recycling.

Lawrence Berkeley National Laboratory

A circular economy requires products to be designed so that at their end of life their constituents can be recovered and either reused or repurposed. Batteries, which are playing a prominent and widespread role in an increasingly decarbonized world, present a challenge to such designs. For example, current electrode binders require expensive processes including shredding, grinding, pyrolysis, or organic solvents to recover materials, which can release toxic gases that need to be recovered. Given the burgeoning worldwide demand for energy storage, and the necessity to recover and reuse battery materials on a large scale, a simpler, less expensive, and more environmentally friendly approach is needed.

Our team has developed a dissolvable ionic crosslinked polymer (DCIP, or Quick-Release *Binder*) that meets this challenge. This novel binder, which is a drop in replacement for current binders, can be used to bind electrode (anode or cathode) materials and provides comparable performance at one-tenth of the cost of current commercial binders. The three-dimensional network structure of DICP is formed by crosslinking two chemicals through a carboxy-amino ionic interaction. This interaction is pH-controlled, and therefore, the crosslinking is readily dissociated in basic condition (i.e., an aqueous sodium hydroxide solution), thus providing a plausible approach to recycle common materials such as LiFePO₄ cathode (LFP) and graphite anode through a simple washing method using water. (This binder may work with NMC cathodes, which are amendable to water-based processing.) The threedimensional network structure of DICP enhances the mechanical integrity of the electrodes for high performance cells. Therefore, with the application of this robust binder, the lithium (Li)-ion batteries achieve excellent electro-chemical performance. Figure 1 shows the fabrication of a graphite/LFP battery with the Quick-Release binder, as well as a process demonstration. The recycled cathode, anode, and binder components can be re-fabricated into new cells that exhibit capacity comparable to fresh materials. The solvent employed in both the electrode preparation and the recycling processes is merely low-cost distilled water.

Therefore, this binder may support green battery production and recycling, and a circular economy. This could provide a major advantage compared to some current conventional binders, which use less environmentally friendly organic solvents for battery construction.

Future work will test this new binder in larger pouch cells to investigate any scale up issues and potentially the use of other, less corrosive, bases in the processing with this binder.



Figure 1. Schematic illustration of battery fabrication and recycling using the Quick-Release Binder. The lithium iron phosphate (LFP) cathode material and graphite (Gr) anode material are fabricated into cathode and anode sheets, which are then cut to assemble cells for cycling test. Upon recycling, the cells are disassembled, and the LFP cathodes and graphite anodes are individually treated with high pH aqueous solution to separate the electrode materials from the current collector foils. The LFP and graphite electrode materials are retrieved from their aqueous suspensions.

Page 12 | Electrochemical Energy Storage Technical Team



Abundant Cathodes

In this work, we developed an in-situ fluorination method that produces high-energy LMR cathodes with significantly reduced side reactivities and improved cycling performance.

Lawrence Berkeley National Laboratory

Key to sustainable energy storage is the development of lithium-ion battery (LIB) cathodes using earthabundant elements. Lithium and manganese-rich (LMR) layered oxides are one of the leading contenders in this category. However, despite years of development, performance issues, such as capacity decay, voltage fade, and impedance rise during cycling, remain as major roadblocks. Here we show that a new fluorination approach can address some of these challenges.

Many fluorination processes use LiF as the fluorine source, which often leads to impurities in the final product. We have developed a molten-salt approach where we use fluoride salt mixtures with a low fluoroacidity to improve fluorination efficacy and reduce apparent impurities in the final product. The treated cathodes show improved performance, particularly reduced oxygen gas evolution, decreased side reactions with electrolyte, higher energy density and energy retention. Figure 1 shows the results cobalt (Co)-free fluorinated using LMR. Li_{1,2}Ni_{0,2}Mn_{0,6}O₂ (referred to as LNMO). We used large micron-sized single-crystal samples (Figure 1b inset) to demonstrate the effect of in situ fluorination. Using the optimized F precursor, we obtained phase-pure fluorinated LNMO samples, including LNMO-F1, LNMO-F2.5 and LNMO-F5 with a fluorination level of 0.5%, 0.125%, and 2.5% (Figure 1a). In Figure 1b, fluorinated LNMO shows additional redox processes at ~2.7, 4.7 and 4.75 V, indicating the involvement of a high-voltage spineltype (LiNi_xMn_{2-x}O₄) component. These features lead to increased energy density and better energy retention. The initial discharge energies were \sim 705, 725, 715, and 730 Wh/kg for LNMO, LNMO-F1, LNMO-F2.5, and LNMO-F5 cathodes. After 50 cycles, the specific energies were ~ 695, 650, 725 and 775 Wh/kg, with an energy retention of ~ 98%, 90%, 102% and 106% (Figure 1d). *Operando* diagnostics revealed decreased oxygen activities in fluorinated LMR and reduced side reactions at high voltages. This strategy is expected to be applicable to LMR with other compositions, sizes and morphologies. Future work will investigate the cost impact of this technology (including the ability to recover and reuse the molten salt).





2023 U.S. DRIVE Highlight Investigating High-Voltage Lithium Cathode-Electrolyte Interfaces

Researchers characterize nanocomposite, earth-abundant, cyclable manganese cathodes.

Lawrence Berkeley National Laboratory

"Li₄Mn₂O₅" is a nanocomposite of Li₂O and a disordered rock salt with composition Li_{4-x}Mn₂O₅ made by reactive ball-milling. It is notable for very high initial discharge capacities in lithium half-cells, which can exceed 300 mAh/g, depending on current density and voltage limits used. The origins of the anomalously high capacity were, until this study, not clear. Comprehensive spectroscopic characterization using resonant inelastic X-ray scattering mapping, (m-RIXS) X-ray Raman (XRS), and X-ray absorption spectroscopy (XAS) showed conclusively that reversible oxygen redox does not occur in this system and that the capacity can be entirely explained by decomposition of Li2O upon charge and over-reduction of manganese (Mn) below +3 upon discharge. Unfortunately, Li₄Mn₂O₅ evolves oxygen at high potentials and undergoes structural changes, as well as rapid capacity and voltage fading, when cycled over a wide potential range (Figure 1). Narrowing the voltage window to improve cyclability greatly compromises energy density. Likewise, fluorination, which improves the behavior of other disordered rock salt electrode materials, has only a marginal benefit. In contrast, milling Li₄Mn₂O₅ with $LiMn_2O_4$ greatly improves cvcling spinel performance. While capacity is slightly lowered, first cycle coulombic efficiency and cycle life is improved as spinel content is increased. The best compromise between cycling behavior and capacity is exhibited by the material made with a ratio of 6.5:3.5 Li₄Mn₂O₅:spinel. This material still gives over 250 mAh/g with minimal capacity and voltage fading. Oxygen evolution at high states-of-charge is also greatly reduced. Future work will focus on understanding and mitigating Mn dissolution in Li₄Mn₂O₅ and the spinel-modified material



Figure 1. (a-g) Charge and discharge profiles over five cycles for (a-g) Li₄Mn₂O₅ and spinel-modified Li₄Mn₂O₅ in the indicated ratios. (h) Capacity as a function of cycle number for the same cells.

Page 14 | Electrochemical Energy Storage Technical Team



2023 U.S. DRIVE Highlight Fast Diagnosis of Li-ion Battery Health from High-Rate Data using Artificial Intelligence

Age-informed electrochemical models used in conjunction with machine learning determine battery state-of-health physics during high-rate cycling.

National Renewable Energy Laboratory and Idaho National Laboratory

Under the U.S. Department of Energy's physicsbased machine learning program, the National Renewable Energy Laboratory (NREL) and Idaho National Laboratory (INL) are developing methods to rapidly diagnose lithium (Li)-ion battery state-ofhealth (SOH) during high-rate cycling, specially 10 minute fast charge and two hour discharge. The goal is to quickly determine the severity of battery aging modes (e.g., loss of active material [LAM], loss of lithium inventory [LLI]) without taking the battery out of commission for a standard slow-rate, fullcapacity evaluation, which can take up to 40 hrs.

To develop online SOH diagnostics, NREL's battery physics models are combined with INL's machinelearning tools. Figure 1 illustrates the overall workflow. First, an electrochemical battery model is developed that can predict high-rate battery performance of aged cells. Second, features, such as the incremental capacity during charge, are extracted from the synthetic data generated by the electrochemical model. Third, the synthetic data is used to train a machine-learning algorithm to associate how the high-rate voltage response should change under different aging conditions. Fourth, after training the machine-learning model on synthetic data, the model is tested on real cells.

The new state-of-health diagnostics method, (Weddle, Journal of Power Sources, 2023), accurately determines battery state-of-health physics and compares well with slower check-up test methods. Compared to the standard 40-hour fullcapacity diagnostic, the new method provides a 10x speedup in quantifying failure modes and enables earlier life projections using less data.

Importantly, the new method can analyze the cell SOH each time the battery is used and can use high rate and rest information for failure mode identification, quantification, and projection. The new accelerated check-up tool is expected to improve battery safety by providing a consistent indicator that offers a faster method for assessing aged cells. Future work will investigate the applicability of this method to full pack diagnostics.



Figure 1. Process to develop an online battery state-of-health monitor by using electrochemical models and machine learning. Validation data is from single-layer pouch cells aged under 10-minute fast-charge and 2-hour discharge cycling protocol.

Page 15 | Electrochemical Energy Storage Technical Team



2023 U.S. DRIVE Highlight Silicon Anode Technology for Next-Generation Lithium-Ion Batteries

A novel processing method is developed for production of silicon nanoparticles.

National Renewable Energy Laboratory

The National Renewable Energy Laboratory (NREL) has developed a novel processing technology for silicon that could disrupt current lithium-ion battery (LIB) technology. Conventional LIBs use graphite anodes-a non-domestic, critical material-that limit cell performance. Silicon can be a drop-in replacement for graphite, and it offers over 10 times the lithium storage capacity compared to graphite. NREL's silicon nanoparticle (Si NPs) production process is similar to a process used in the semiconductor chip and solar cell manufacturing industries. The Si NPs are then coated with molecules that transform them into a form compatible with conventional battery electrode manufacturing. These Si NP-based anodes are free from critical materials and could be manufactured entirely with a U.S. domestic supply chain.

This advance was made possible by years of work to understand failure processes in silicon-based LIBs. These studies resulted in strategies to engineer silicon that led to the development of NREL's patented Si NP molecular coating technology, which can be seen clearly in images of the Si NPs with and without the molecular coating (Figure 1). Detailed studies¹ have shown this processing methodology:

- 1. Stabilizes the Si NP active material against degradation during handling in air, potentially simplifying manufacturing.
- 2. Enables full access to all the Si NP active material in the electrode during the first lithiation cycle, enhancing the available specific capacity.
- 3. Encapsulates the Si NP active material in an organic matrix material, mitigating cycle and calendar life performance declines.

Research-scale coin cells (3mAh capacity) achieve impressive cycling life (nearly 1000 cycles) and capacity (over 2000mAh/g) metrics, Figure 2.

Preliminary cost modeling finds that a scaled PECVD production process would approach the \$5-\$15/kg U.S. Department of Energy target for active material costs.

Calendar life—the major performance metric limiting commercial adoption of silicon-based LIBs—is under active investigation. In addition, the team plans to test performance of these NP-Si based is full single layer pouch cells.



Figure 1. Images of Si NPs (a) before and (b) after applying a molecular coating and processing into an electrode.



Figure 2. The cycle life of batteries containing a Si NP-based anode and an NMC811 cathode achieves U.S. DRIVE goals of cycle life >1000 with an anode available specific capacity >2000 mAh/g at a nominal voltage of 0.01 V vs Li/Li⁺.

¹ <u>https://doi.org/10.1039/D2TA08935A</u> and

https://doi.org/10.1002/aenm.202203921.



2023 U.S. DRIVE Highlight Carbon Coatings Improve the Cycling Performance of Disordered Rocksalt Cathodes

Graphite coatings promote a robust electronically conductive network and stabilize the cathode/electrolyte interface for high voltage disordered rocksalt cathodes.

Oak Ridge National Laboratory

Lithium (Li)-excess disordered rocksalt (DRX) oxides and oxyfluorides are a promising class of next-generation Li-ion cathodes due to their high specific energy (≥800 Wh/kg) and compositional flexibility. More specifically, DRX formulations containing earth abundant transition metals (e.g., manganese [Mn] and titanium [Ti]) can reduce reliance on critical and expensive materials such as cobalt (Co) and nickel (Ni).

Despite their promise, DRX cathodes typically require large amounts of conductive carbon additive (20%-30%) to obtain high capacity and stable cycling. This approach compromises the electrodelevel energy density and exacerbates electrolyte breakdown, which yields a resistive cathode/electrolyte interface. As such, improved understanding of how different carbon additives impact the structure and performance of DRX cathodes is needed.

To address these issues, researchers at Oak Ridge National Laboratory working in the DRX+ Consortium have developed a mechanical milling process to apply conformal graphite coatings to DRX cathodes. Figures 1a-1b compare cycling performance of Co/Ni-free DRX cathodes (Li_{1,2}Mn_{0.5}Ti_{0.3}O_{1.9}F_{0.1}) containing either a graphite coating or one of two carbon blacks. At a moderate carbon loading, the carbon black-based electrodes exhibit high initial capacity (ca. 250-300 mAh/g, compared to 200mAh/g for current commercial cathodes) but rapidly fade over 50 cycles. On the other hand, the graphite-coated DRX (10%, ~20 micron thick conformal coating) shows superior cycling stability with 85% capacity retention after 45 cycles (vs. 56%-58% retention for cells with carbon black).

A suite of characterization tools (e.g., electron microscopy, Raman spectroscopy, and mass spectrometry) was employed to assess differences in electrodes containing graphite coatings vs. traditional carbon blacks. Collectively, these results show that carbon blacks agglomerate on the DRX surface which yields precarious electrical contacts throughout the electrode (see Figure 1c). On the other hand, the graphite coating provides two key advantages by protecting the DRX surface from parasitic reactions (e.g., electrolyte oxidation) and providing a robust conductive network that can withstand repeated volume changes during cycling. Overall, these results demonstrate the efficacy of conductive coatings to improve the performance of DRX cathodes. Ongoing work is focused on optimizing the graphite coating, reducing the carbon content to $\leq 5\%$, which is critical for practical devices, and investigating scale up issues.





2023 U.S. DRIVE Highlight Advancing All-Solid-State Lithium-Sulfur Battery through Materials and Interfacial Innovations

This work demonstrates a highly conductive solid electrolyte, engineered cathode structure, and regenerative solid-electrolyte interface to advance earth abundant cathode and high energy cells.

Pacific Northwest National Laboratory

Developing next-generation battery technologies that are more energy-dense and cost-effective is crucial for the widespread adoption of electric vehicles. Sulfur (S) is a promising cathode for nextgeneration lithium batteries due to its high theoretical capacity (1670 mAh/g vs. 220 mAh/g for transition metal oxides), natural abundance, and extremely low cost compared to conventional layered oxide cathodes. However, current lithiumsulfur (Li-S) batteries suffer from low usable capacity and short lifespan rooted in S dissolution. Switching from a liquid to a solid-state electrolyte could potentially overcome these issues. Yet, allsolid-state Li-S cells have their own challenges such as slow reaction kinetics and unstable interface between the lithium anode and solid electrolyte.

A team at Pacific Northwest National Laboratory (PNNL) has developed an integrated approach that improves the performance of all-solid-state Li-S batteries (Figure 1). They have developed a Li compatible solid-state electrolyte (SSE) with high ionic conductivity (>5 mS/cm at room temperature) and integrated it with engineered carbon materials to host the S. Through rational design of the Scarbon-SSE triple-phase, the team achieved neartheoretical S capacity (~1600 mAh/g) in Li-S batteries, with a high S mass loading (>10 mg/cm²) (Figure 1c). This lays a solid foundation for the further fabrication and manufacturing of highcapacity electrodes (up to 16 mAh/cm²) and highenergy batteries.

Moreover, the S cathodes deliver superior power performance. Figure 1c exhibits the cell capacities as a function of current densities, demonstrating both high-rate capability and electrode robustness. Based on the team's preliminary results, the engineered cathodes (~1500 mAh/g at 5 mg/cm²) have a great potential to meet a cell-level energy of a 500Wh/kg in a 5Ah Li-S pouch cell using a 30 μm SSE separator, and 37.5 μm thick Li (Figure 1b).

The improved stability of the developed SSE towards lithium metal also allows for stable cycling of allsolid-state Li-S cells. At 2 mAh/cm² capacity, the allsolid-state Li-S coin cells have demonstrated over 250 cycles without capacity decay or failure (Figure 1f). The team is now working on enhancing the cycle life of all-solid-state Li-S batteries of further increased S loading to achieve high energy goals in prototype pouch cells.



Figure 1. (a, b) Schematic and cell energy estimation based on experimental inputs. (c, d) Discharge profile (10 mg S/cm^2) and rate capability of cell (3.7 mg S/cm^2). (e, f) Charge/discharge profiles and long cycling of all-solid-state Li-<u>S coin cell (1.5 mg S/cm^2). all cells were tested at 20°C.</u>

2023 U.S. DRIVE Highlight Enabling Fast-Charging in Solid-State Batteries

Mechanical defects in solid-state batteries influence fast-charging capability.

SLAC National Accelerator Laboratory & Stanford University

Solid-state batteries promise high-energy density and enhanced safety. In particular, garnet solid electrolyte is chemically compatible with lithiummetal and thus may enable a safer and energy-dense lithium-metal based battery. One major challenge for garnet solid-state battery is fast charging capability. Short-circuiting resulting from lithium intrusion into the solid electrolyte is a major failure mechanism that makes fast charging challenging with this system.

SLAC National Accelerator Laboratory and Stanford University have developed a mechanistic understanding of short-circuiting in garnet solidstate batteries (Figure 1). By using in-situ scanning electron microscopy combined with an electrical microprobe, we have investigated the probability of short-circuiting at the nanoscale level. We discovered that, in the absence of mechanical defects, extraordinary current density, on the order of 10,000 mA/cm², can be achieved without short circuiting. When local mechanical defects are present (e.g., dents, scratches, etc.), the critical current density at which short-circuiting occurs decreases substantially. Specifically, the average local critical current density decreases from 5 A/cm² to 1 A/cm². Our work highlights the critical importance of reducing mechanical defects at the solid electrolyte surface during cell manufacturing, establishing a causal link between defects and fast charging.

We have also developed ultrathin coatings to improve the surface mechanical properties to make solid electrolytes more resistant towards mechanical failure. Specifically, ultra-thin silver (Ag) doping (obtained via annealing Ag metallic thin film) increases the mechanical toughness and increases the critical current density. We expect the mechanistic understanding of shortcircuiting and mitigation by surface treatment will contribute to improved approaches to fast-charging garnet-based solid-state batteries with high safety and energy density.



battery driven by mechanical defects. Reproduced from McConohy et al. Nature Energy 8, 241 (2023).



2023 U.S. DRIVE Highlight

Transport-Regulating Polymer Coating to Improve the Cyclability of Lithium-Metal Batteries

A polymer coating that transports salt while blocking the solvent at the lithium-metal anode can improve battery cyclability.

Stanford University

Lithium (Li)-metal batteries are promising candidates for next-generation energy storage devices, particularly in the context of electric vehicles, owing to their high energy density. However, the inefficiencies in Li-metal plating and stripping during cycling has been one of the main obstacles impeding commercialization. Researchers at Stanford University have invented a polymer coating for the Li anode that improves the battery cyclability by more than two-fold while employing various common electrolytes (e.g., ether, carbonate, and fluorinated ether electrolytes).

The high reactivity of Li-metal anodes with electrolytes often leads to formation of an unstable interfacial layer, the solid electrolyte interphase (SEI). Unfortunately, this SEI layer often fails to passivate the Li-metal surface or facilitate uniform Li deposition. Consequently, continuous side reactions between Li and electrolytes, whisker-like Li deposition, and development of inaccessible Li, all occur during cell cycling.

Alternatively, our team has designed a polymer coating (applied by standard coating process, such as blade coating or spray coating) capable of regulating salt and solvent transport at the Li anode interface. The dual-function polymer coating, denoted as SP², is engineered to selectively block solvents while facilitating the transfer of salt molecules, resulting in formation of a salt-derived SEI layer (Figure 1a). Several common electrolytes, including ether, carbonate. and fluorinated carbonate-based electrolytes demonstrated improved Li cycling efficiency when using the polymer coating (Figure 1b). Further, employing the SP² polymer coated Li anode in full battery with either carbonate or fluorinated ether electrolytes exhibits enhanced cyclability by a factor of greater than two (Figure 1c and 1d).

The concept of introducing a regulating polymer coating at the Li anode presents an opportunity for researchers to harness the potential of polymer chemistry to enhance battery cyclability. Furthermore, this strategy may hold promise for extension to other battery systems, such as sodium metal.



Figure 1. (a) Scheme of a regulating SP² polymer coating at the Li anode that blocks solvents while transports salts. (b) Compared to the bare ones, Li metals with SP² coating exhibit improved Li cycling efficiency when using different electrolytes. Tests of full cells with SP²-coated Li anodes indicated improved cyclability using (c) carbonate and (d) fluorinated ether electrolytes.



2023 U.S. DRIVE Highlight High-Entropy Electrolytes for Lithium-Metal Batteries

A new class of electrolytes, called high-entropy electrolytes, employs entropy to improve electrolyte properties and enables fast charging and long-lasting lithium-metal batteries.

Stanford University and SLAC National Accelerator Laboratory

The electrolyte is a crucial part of the lithium-metal battery that impacts the fast-charging capabilities, safety, and particularly cycle life. Recent advances in electrolyte engineering have greatly improved cyclability by enhancing electrochemical stability at the electrode interfaces. Improving cycling stability, however, seems to compromise ionic conductivity that directly hampers the fast-charging capabilities, and concurrently achieving stability and conductivity has been challenging.

Scientists at Stanford University and SLAC National Accelerator Laboratory designed a novel class of electrolytes called high-entropy electrolytes (HEEs) that improves ionic conductivity without sacrificing cycling stability. By utilizing a variety of solvents, up to five different solvents, the solvation entropy of the electrolyte was observed to increase (Figure 1a). Solvation entropy was shown to play a critical role in modulating the ion clustering behavior within the electrolyte. HEEs have smaller ion clusters that allows for faster ion transport (Figure 1b). Researchers observed that HEEs possess more than 100% improvements in ionic conductivity compared to the conventional low entropy counterparts (Figure 1c). Improved ion transport allows for a more uniform Li⁺ concentration profile and lithium deposition morphology (Figure 1b). In addition, the superior ionic conductivity enabled cycling at fast charging conditions of up to 2C. Faster charge rates will be investigated through improved cells designs.

In this study, HEEs were designed to improve both cycling stability and ionic conductivity. This discovery not only improved fast-charging and cycle life of lithium-metal batteries, but also opened up a new space of HEEs that can potentially support further advancement towards practical lithiummetal batteries in the future. Future work may involve optimizing HEEs for lithium-ion chemistries, and to investigate cost and mass manufacturing of these solvents.



Figure 1. (a) Schematic showing that increasing molecular diversity increases the solvation entropy of the electrolyte. (b) Illustration showing that HEE has smaller ion clusters and superior ion transport. (c) Ionic conductivity doubles for the HEE (labeled EL5) compared to conventional electrolytes (EL4 and 4). (d) HEE enables stable cycling at fast charging conditions.

Fuel Cells

2023 U.S. DRIVE Highlight Reducing the Cost of Compressed Hydrogen Storage

Reduced compressed hydrogen storage system costs enables accelerated mass deployment of hydrogen fuel cell electric vehicles.

Hexagon Agility

Hexagon Agility's multifaceted optimization strategy to develop reduced cost, high-strength carbon fiber leads to further reductions in onboard hydrogen storage system costs.

The high cost of hydrogen storage tanks is a significant barrier to the widespread adoption of fuel cell electric vehicles. The tank's carbon fiber overwrap accounts for more than half of the total hydrogen storage system cost. Reducing the cost of high-strength carbon fiber is critical to improving tank performance and cost.

In 2021, DOE implemented a two-phase funding program to enable a 50% reduction in carbon fiber costs in five years. Four projects, comprising teams from industry and academia, were selected in the first phase to develop lower cost carbon fibers and, by extension, hydrogen storage tanks. At the end of the two-year Phase 1 period, each team's progress was evaluated based on the properties and projected cost of their carbon fiber, as well as the projected performance and cost of their hydrogen storage system. Achievements in each of these components highlight the work being done to reduce carbon fiber cost, as well as storage tank mass and cost.

During Phase 1 of the project, the team led by Hexagon Agility used a multi-track approach to develop carbon fibers with greater than 725 ksi tensile strength and greater than 35 Msi tensile modulus, exceeding the properties of the widely used Toray T700S carbon fiber. The team's projected carbon fiber cost is between \$15/kg and \$20/kg, which represents a more than 20% reduction in carbon fiber cost compared to T700S. The team also projected tank mass reductions leading to a lower projected tank cost of \$12.8/kWh (Figure 1) and an improved projected gravimetric capacity of 1.7 kWh/kg. Hexagon Agility's team was down selected as the most promising project and will continue their carbon fiber and storage system optimization efforts during the three-year Phase 2 period. Further improvements in carbon fiber spinning and conversion, fiber surface treatment, and tank design provide avenues for additional reductions in carbon fiber and storage tank cost, as well as improved storage tank performance. Their Phase 2 work will also address sustainability considerations via the recovery and reuse of high-quality carbon fibers at the storage tank's end-of-life.



2023 U.S. DRIVE Highlight

Reducing the Cost of Owning Hydrogen Fueled Vehicles Assessment of heavy-duty fueling components and protocols points the way to better safety and lower

Assessment of heavy-duty fueling components and protocols points the way to better safety and lower costs.

National Renewable Energy Laboratory

National Renewable Energy Laboratory's (NREL) comprehensive assessment of heavy-duty (HD) fuel cell vehicle (FCEV) hardware and fueling protocols helps stakeholders minimize the total cost of ownership (TCO) and ensure functional safety by optimizing station and vehicle design.

NREL's high-flow hydrogen fueling testing and research facility has generated high-flow fueling data, which will enable the timely development of fueling protocols and standards. NREL is one of the first to fully implement the SAE J2601-5 fueling protocol, which is a hardware and model validation challenge. NREL completed a 70.5 kg fill in seven minutes into a HD vehicle simulator tank array, meeting safety limitations related to tank array pressure and temperature and supported by advanced wireless communications of real-time fueling data between the fueling system and the tank array.

The fueling research facility comprises a heavy-duty research dispenser, heavy-duty vehicle storage simulator, high-capacity hydrogen chiller system, and 665 kg of bulk gas hydrogen storage (see Figure 1.). At the design conditions (700 bar at -40°C). The facility can transfer precooled pressurized hydrogen gas at an average flow rate of 10 kg/min (27 kg/min peak), which is sufficient to fill a heavy-duty truck in seven minutes for a range of 750 miles. A team led by NREL completed the construction of the facility, leveraging comprehensive modeling tools (e.g., computational fluid dynamics and hydrogen filling simulation (H2FillS)) and existing hydrogen infrastructure at the site. This is a large step forward from dispensers for light-duty fuel cell vehicles, which typically fuel at an average flow rate of less than 2 kg/min for a total of only 10 kg of fuel.

The accomplishments of this project can be grouped into three categories: hardware, modeling, and analysis. NREL has implemented station hardware improvements, evaluated refueling hardware with new HD fast flow fueling protocols and advanced communication concepts, identified key technology informed codes and standards gaps, and organization on project progress. These codes and standards reduce the risk of entering the market and enable lower cost through higher production of standard parts. As for modeling, the project team modified H2FillS for HD applications and performed numerous CFD simulations on hydrogen tanks. Lastly, the analysis team utilized the combined model structure to perform technoeconomic and TCO analyses on industry-identified metrics and scenarios and performed sensitivity analyses on two HD fast flow fueling protocols: SAE J2601-5 and PRHYDE.

NREL's project team is assisted by several stakeholders including industrial partners Chevron and NextEnergy (liaison for Air Liquide, Hyundai, Nel Hydrogen, Nikola, Shell, and Toyota), as well as Argonne National Laboratory.



Figure 1. Heavy-duty vehicle simulator tank array (left) and dispenser communication module (right)

Materials



2023 U.S. DRIVE Highlight Manufacturing Demonstration of a Large-scale, Multi-Material Passenger Vehicle Sub-system

A unique composite-intensive multi-material body-in-white intended for mass production

Clemson University, University of Delaware, Ohio State University, and Honda

Researchers at Clemson University, the Center for Composite Materials at the University of Delaware, Honda Development and Manufacturing of America, and Ohio State University (OSU) are manufacturing a thermoset composite intensive multi-material body-in-white intended for mass production to replace a current baseline steel body-in-white (Figure 1). Project objectives include:

- 4. To achieve a weight reduction of 160 lbs.
- 5. To ensure zero compromises on performance targets such as crash performance, noise/vibration/harshness durability, etc.
- 6. To limit cost increment to \$5/lb of weight saved.
- 7. To achieve annual production of 200,000 vehicles.
- 8. To incorporate state-of-the-art multi-material joining processes, including ultrasonic additive manufacturing (UAM).
- 9. To maintain OEM's spot-welding-enabled factory assembly process for composite-intensive multi-material parts.
- 10. To utilize recycled carbon fiber to enable sustainable light-weighting

The team is advancing the production of snap curebased thermoset composites reinforced with virgin and recycled carbon fibers through wet compression molding (WCM) and high-pressure resin transfer molding (HPRTM). This approach is set to meet weight reduction and performance benchmarks while targeting production efficiency with cycle times reduced to under two minutes. At the core of our innovation is implementing a patented Ultrasonic Additive Manufacturing (UAM) process developed in collaboration with Honda and OSU. This process preserves the conventional spotwelding techniques, aligning seamlessly with existing OEM assembly processes. This integration is contrary to prevalent industry methods that rely heavily on adhesives to include thermoset composites, which typically necessitate a substantial overhaul of OEM assembly lines. Lastly, the team developed a parametric cost model and proprietary factory layout simulations to accurately forecast production costs for thermoset components with UAM joints, promoting their rapid integration into manufacturing processes.

Our deliverables to date are being made possible by creating a digital lifecycle that uses proprietary userdefined subroutines and commercial finite element analysis software to couple manufacturing processes with mechanical performance. The pathway is designed to predict changes in composites and joint microstructure and couple these to mechanical simulation to help predict mechanical performance. The pathway has been validated at a coupon level. It is currently being experimentally validated at a subcomponent level with quasi-static and dynamic experiments, and a full-scale vehicle crash will be validated next year.



Figure 1. Overview of the composites-intensive multimaterial body-in-white intended for mass production and assembled using spot-welding technology.

2023 U.S. DRIVE Highlight Modeling Damage Accumulation in Corrosion of Polymeric Adhesives

Predicting damage induced by any combination of thermal loads, moisture, UV, vibration, and stretch.

Michigan State University

Corrosion in polymeric adhesives poses a significant threat to the joints of electrical and structural vehicle components. Environmental factors leading to adhesive degradation can drastically impact component performance and, as a result, vehicle reliability. Failures caused by corrosion result from various factors like thermal degradation, oxidation, hydrolysis, radiation, and moisture, combined with aging and fatigue. Accurately predicting the service life of adhesives could not only enhance their usage over mechanical fasteners but also save 20%-40% in costs associated with repairing unexpected failures.

In collaboration with Robert Bosch GmbH, Michigan State University has created a combined approach involving experimental, computational, and analytical methods to develop a theoretical platform (Figure 1). This platform predicts how polymeric adhesives degrade over time under various environmental and mechanical pressures. We validated this platform using a comprehensive series of tests on different types of adhesives, including epoxy, silicone, and polyurethane. For the first time, our platform predict concurrent damage builds up in adhesives for any combination of mechanical & environmental stresses during certain service-life.

Before, no commercial tools were capable of addressing durability issues caused by concurrent degradation in polymeric materials. To address this issue, the developed modeling technology was released to Endurica, a lead provider of fatigue models for elastomers, and Karax LLC, a lead provider of machine-learned models for the degradation and durability of polymeric materials.

We developed computational models that combine several degradation pathways—thermal, oxidative, hydrolytic, and photo-induced aging—into a unified constitutive/data-driven framework. This method is a departure from traditional approaches, which usually focus on single degradation factors, providing a more comprehensive view of material durability. Achieving average error below 10%, validation efforts showed the model's ability to predict the service-life of most common adhesives from DOW, 3M, and Parker Lord used in automotive industry. The platform can guide the selection, condition monitoring & selection of adhesives.



Figure 1. Hybrid platform for Multi-stressor Aging prediction and its impact on adhesive performance over time. Experimental data, developed models and codes are publicly available. Commercial codes are also developed for Fatigue (Endurica.com), and lifetime aging/durability (Karax.us).

2023 U.S. DRIVE Highlight Changing the Design Rules of Rubber to Create Better Wearing, Lighter Weight, More Fuel-Efficient Tires

Improving rubber composites for electric vehicle tire tread using functionalized carbon nanotubes.

Molecular Rebar Design, LLC

Electric vehicles (EVs) are heavier than their internal combustion engine counterparts, and produce higher, more instantaneous torque, which reduces EVs tire lifetimes by 30%-40%. Tires wearing more quickly increases cost of ownership for EVs, creates more micro-rubber (comparable to micro-plastic) pollution per mile driven, and creates larger quantities of tires for disposal. Using chemically functionalized MOLECULAR REBAR[®] (MR) carbon nanotubes, developed with funding from U.S. Department of Energy award DE-SC0021823, to produce a new tire tread composite material resulted in numerous benefits:

- Improved tire tread wear resistance and lifetime
- Reduced composite density, reducing tire weight
- Improved rolling resistance, corresponding to improved fuel/energy efficiency
- Reduced rubber particulate emissions
- Other key performance needs are maintained, not sacrificed as is typical, such as tread stiffness and wet grip.

Rubber tire tread consists of many ingredients rubber, fillers, antioxidants, crosslinking chemicals, etc.—that are mixed to form a rubber compound. For some tires, carbon black is the preferred reinforcing filler, while for more efficient tires, like those for EVs, silica coupled with silane is the preferred filler to maximize wet grip and energy efficiency. Silica loadings in tire treads are 30%-40% by weight, with higher loadings of silica being pursued for improved wear resistance.

Replacing up to 50% of the silica content, with a much smaller replacement loading of MR, reduces tire tread density, and improves properties. This is achieved through the invention and use of individualized carbon nanotubes functionalized with hydroxyl and carboxyl groups chemically bound with an organosilane and the rubber itself: silane-coupled MR. The dispersion and individuality of the nanotubes provides superior reinforcement compared to typical fillers, while the coupling improves MR-rubber interaction. Molecular Rebar Design, LLC (MRD) developed an easy-to-use synthetic polymer masterbatch product form which is usable in the existing tire manufacturing process with minimal changes.

To prove and commercialize this tire technology, MRD is working with Goodyear to develop and build EV tires for vehicle testing to demonstrate improved laboratory properties translate to field results. Figure 1 shows the new balance of key tire tread properties using MR vs. state-of-the-art tread, designed by Goodyear for EV applications, and optimized to improve both efficiency and lifetime. Typically, improvements in one tire tread property, like wear resistance, result in a detrimental effect on another tire tread property, like rolling resistance. With silane-coupled MR. а simultaneous improvement in wear resistance and rolling resistance is achieved, while wet grip is retained, expanding tire performance without sacrifice.



Page 28 | Materials Technical Team



2023 U.S. DRIVE Highlight Bio-based, Inherently Recyclable Epoxy Resins to Enable Facile Carbon-Fiber Reinforced Composites Recycling

Redesigned resin enables the beneficial re-use of carbon fiber.

National Renewable Energy Laboratory

Despite the promising benefit of today's carbon fiber reinforced composites (CFRCs), they are often limited in use due to high cost, high associated emissions with manufacture, inability to be reused, and brittle nature. To further incentivize the use of CFRCs, the team at the National Renewable Energy Laboratory (NREL) has aimed to design bioderivable and recyclable resins which lower the emissions associated with the first life of the CFRCs while enabling second life use.

During previous years of this work, the team at NREL demonstrated and a polyester covalently adaptable network (PECAN) resin made from the reaction of epoxies and anhydrides that could exhibit comparable performance to today's epoxy-amine CFRCs. Additionally, the PECAN resin exhibited a comparable cost to today's CFRCs while emitting 40+% less greenhouse gas emissions. This work was recently published in Matter for glass fiber composites (DOI: 10.1016/j.matt.2023.10.033).

Importantly, the use of the PECAN resin enables both the thermoforming of the CFRCs and their recovery via methanolysis. In both cases, the alignment of the carbon fiber (CF) can be maintained and thus the thermomechanical properties can be maintained over multiple material lives. Subsequent technoeconomic and supply chain analysis (Figure 1A) reveal that this approach can result in >90% savings relative to the first life of the CF or CFRC. In the base case, no co-product or resin is recovered and only the CF is reclaimed; while in the MHHDP Co-product case, the anhydride reclaimed. hardener is Additionally, the thermoforming (which only uses heat and pressure) results in greater reductions.

Overall, this work demonstrates that recyclable-bydesign and bio-derivable resins can address some of the issues associated with CF and CFRC use.





2023 U.S. DRIVE Highlight A Novel Manufacturing Process of Lightweight Automotive Seats

Integration of additive manufacturing and reinforced polymer composite.

Oak Ridge National Laboratory and Ford Motor Company

This project aims to develop a lightweight seatback of a vehicle using a novel hybrid manufacturing process for metal/polymer composite structures. Metal/polymer composites consist of low-density, high-strength composites with ductile and tough metals, exhibit superior mechanical properties, including high modulus/strength and specific energy absorption. However, traditional manufacturing processes face challenges due to limited design freedom, lack of control over fiber orientation, and poor interfacial bonding between dissimilar materials.

We have developed an additive manufacturing (AM) process integrated with a compression molding (CM) process in which we can locally control fiber orientation to manufacture high-performance molded composites that are difficult to obtain with other manufacturing techniques. This project large-scale of discontinuous combined AM reinforced composites with compression overmolding on top of additively manufactured metallic inserts (Figure 1). The resulting hybrid manufacturing process enables the rapid design and production of lightweight automotive seats. The objectives include optimizing project's the lightweight seatback frame through numerical modeling and topology optimization, developing and testing a novel additive manufacturing compression molding (AM-CM) technique, optimizing subcomponents with polymer composite overmolding on metallic lattice structures. fabricating, experimentally testing, and numerically modeling the overmolded parts to assess their mechanical performance.

The novel manufacturing process contributed to weight reduction in car seatbacks and holds relevance for a wide range of structural applications across various vehicle subsystems. The weight reduction of a seatback was achieved with the following specifications.

- Tensile strength of from our method is 76.4 MPa, which is 2-3x higher than that from other joining processes
- Numerical model developed for hybrid structures showed a good agreement with experiments (accurate failure locations and modulus predictions within 20% deviation)
- The flowability of 40 wt% carbon fiber/PA66 polymer composite into metal lattices depends on the lattice depth, leading to successful joining for 4-mm thickness but not enough bonding for 13mm thickness
- Failure analysis shows crack propagation through polymer-metal interfaces and metal lattice strut breakage.
- Topology optimized seatback design with the hybrid structure is 22% lighter and 36% stiffer than conventional metal design.
- The novel manufacturing process developed in this project enabled the fabrication of metal polymer composites with tunable mechanical properties.





2023 U.S. DRIVE Highlight Insights into Creep Behavior of Cast Aluminum Alloys Using *in-situ* Neutron Diffraction

Developing lightweight, creep-resistant aluminum alloys for energy efficiency.

Oak Ridge National Laboratory and Northwestern University

Lightweight, creep-resistant aluminum (Al) alloys are essential for enhancing the energy efficiency of multiple types of vehicles. Al alloys with creep resistance in the 300°–400°C temperature range can improve the energy efficiency and reduce the weight of internal combustion engines. Electrical conductor Al alloys with creep resistance at lower temperatures (up to 200°C) can replace heavier and expensive copper (Cu) alloys enabling energy efficient and affordable electric vehicles with longer driving ranges.

We utilized in-situ creep testing with neutron diffraction at the VULCAN beamline of the Spallation Neutron Source at Oak Ridge National Laboratory to understand the creep deformation mechanisms in cast Al-copper-manganesezirconium (ACMZ) alloys and to enable design of new compositions with enhanced creep resistance. The *in-situ* creep experiments were performed at 300°C on a cast ACMZ alloy and a commercial RR350 Al-copper (Cu) alloy. RR350 is an ACMZtype alloy and contains nickel (Ni) and cobalt (Co) as key additional elements. The RR350 alloy has poor castability and is expensive but exhibits higher creep resistance compared to ACMZ (Fig. 1a). Fig. 1(b, c) show the lattice strains in the strengthening precipitates (θ' -Al₂Cu) measured with the *in-situ* creep tests and compared to the model predictions. The θ' -Al₂Cu lattice strains are indicative of creep activity in grains where higher lattice strains indicate higher creep deformation in the grain bulk. The lattice strain evolution matched well with the model predictions for RR350 but were lower than predicted values for the ACMZ alloy. This result suggested that microstructural regions other than the grain bulk are contributing substantially to the macroscopic creep

strain. Microstructural characterization confirmed that creep strain localized in the soft θ' -precipitatefree zones (PFZs) at the grain boundaries. The RR350 alloy had a lower volume fraction of PFZs which led to its higher creep resistance. The (Ni, Co)rich grain-boundary precipitates in RR350 were more resistant to coarsening resulting in narrower PFZs (Fig. 1e). On the other hand, rapidly coarsening, Cu-rich grain-boundary precipitates and depleted nearby consumed θ' -Al₂Cu precipitates, leading to larger width PFZs with associated lower creep resistance in ACMZ (Fig. 1d).

Based on the insights gained, we developed a new ACMZ alloy containing iron (ACMZ-Fe). Adding Fe formed coarsening-resistant, grain-boundary precipitates which increased the creep resistance of ACMZ-Fe to the same level as RR350 without requiring expensive Ni and Co additions (Fig. 1f). This work demonstrated that *in-situ* neutron creep testing is a powerful tool that can be used to understand and develop creep-resistant Al alloys for automotive applications.



Figure 1. (a). Tensile and compressive creep rates of ACMZ and RR350 at 300°C. Lattice strain evolution in θ' -Al₂Cu during *in-situ* neutron creep testing for (b) ACMZ and (c) RR350 alloys compared to model predictions.² Scanning electron microscope images of crept (d) ACMZ², (e) RR350², and (f) newly designed ACMZ-Fe³ alloy showing extensive PFZs in ACMZ but limited in RR350 and ACMZ-Fe alloys.

² J.U. Rakhmonov et al. Acta Materialia 250 (2023) 118886; ²J.U. Rakhmonov et al. Acta Materialia 228 (2022) 117788; ³US Provisional Patent Application Serial No. 63/559,270.



2023 U.S. DRIVE Highlight <u>High Ve</u>locity (HiVe) Joining: Enabling Multi-Material Joints

A high speed, room temperature joining process to form high strength bonds.

Pacific Northwest National Laboratory

With the advent of advanced materials such as advanced high-strength steel (AHSS), highstrength aluminum, and specialized castings, automakers are pushing the boundaries of innovation to create lighter yet stronger vehicles that improve the driving range and meet durability and safety standards. Multi-material integration, though complex, allows for unprecedented design optimization and improved overall vehicle performance. Joining these advanced materials presents a unique challenge due to their complex microstructures, high strength, and low ductility. They require precise control over heat input to avoid distortion and metallurgical challenges that lower the component's strength. The formation of brittle intermetallic compounds and liquid metal embrittlement at the interface further complicates the joining process, necessitating innovative techniques to mitigate this issue.

Pacific Northwest National Laboratory (PNNL) has developed a novel High Velocity (HiVe) joining process that addresses these concerns, and the total process time is less than 100 microseconds. The two variants of the process HiVe Clinch and HiVe Rivet offers the necessary versatility needed for joining the next generation materials. Figure 1 shows the process flow schematics of these two variations.

During the HiVe process, the punch is propelled at high velocities (more than 120 m/s) to impact the similar and dissimilar multi-material stacks. This action results in plastic deformation and frictional sliding at material interfaces, generating localized increases in temperature and pressure. The localized heating, driven by adiabatic shear instability, fosters the creation of a small region of metallurgical bond, distinguishing it from traditional processes reliant on mechanical interlock or joining methods.

HiVe demonstrated a 1.5x improvement in lap shear strength compared to flow drill screw and more than 7x improvement in strength as compared to traditionally clinched of 6061 joints. The high velocity of the HiVe process demonstrated a significant absence of liquid metal embrittlement (LME) in 3rd generation AHSS joints, a phenomenon occasionally observed in certain resistance spot welds of AHSS. Through this process, we successfully fabricated high-strength joints using PHS1300 grade steel by incorporating a steel fastener at room temperature, predominantly accomplished through steel heating or punching and pre-drilling techniques. These results signify a paradigm shift in enabling the joining of nextgeneration materials through the HiVe process.



Figure 1. Schematics of HiVe Clinching and HiVe Riveting process.



2023 U.S. DRIVE Highlight Hybrid Dispersion Strengthened Aluminum Matrix Composites for Higher Efficiency EV Powertrains

Enhancing wear and mechanical performance of lightweight aluminum composites for replacement of cast iron and steel components in brakes, differential, and structural applications.

Pacific Northwest National Laboratory

The emergence of electric vehicles (EVs) underscores the critical role of lightweighting in offsetting the increased weight from batteries and electrical components to extend driving range. In a modern EV powertrain, 40% of weight saving is possible when steel and cast iron parts are replaced by aluminum metal matrix composite (Al-MMC) parts. In addition, lower wear and corrosion rates of Al-MMC reduces non-exhaust particle emissions from the brake system, which constitutes 59% of road particulate matter emissions.³

Several EV benefits can make the aluminum parts feasible. Regenerative braking in electric/hybrid vehicle operation decreases the amount of energy that must be dissipated by the mechanical brakes by as much as 40%. Reduced brake temperatures and increased service intervals may facilitate a resurgence in the use of Al-MMC brake rotors in EVs.

This project addressed the challenges associated with Al-MMCs and investigated sustainable, lowercost MMCs with matching or better performance to cast iron or steels. TiB₂ was chosen as the reinforcement particles for their lower cost and better wettability with the aluminum matrix. Squeeze casting was chosen for its high quality, costeffectiveness, and scalability. Composite brake rotors were fabricated in collaboration with Loukus Technologies, Inc., Michigan (Figure 1 top). The composites had a hybrid microstructure consisting of submicron-sized in-situ TiB₂ and micron-sized regular TiB₂ powders.

Brake testing of the composite rotors revealed significant outcomes. The coefficient of friction

(CoF) and wear rates of the hybrid composites were notably lower compared to both the control sample (no TiB₂) and the gray cast iron benchmark (Table in Figure 1). Loukus Technologies is now offering the hybrid composite products and the squeeze casting capability developed in this project to their customers for commercialization of Al-MMC brake rotors, which have the potential in decreasing the brake system weight by ~ 15 kg for a typical EV.

Leveraging its solid phase processing capabilities, Pacific Northwest National Laboratory also developed powder metallurgy routes for producing near-net-shape composites like gears for structural applications. These composites exhibited exceptional strength and stiffness values compared to other Al-MMCs.



Figure 1. Casting of the composites is shown in the top left. Aluminum composite and cast iron sub-scale brake rotors in the top right. Brake pad interaction and tribological properties are shown below.

³ Air Quality Expert Group, 2019, "Non-Exhaust Emissions from Road Traffic," Report prepared for Department for Environment, Food and Rural Affairs.

2023 U.S. DRIVE Highlight Machine Learning for Automated Weld Quality Monitoring and Control

Machine learning-based platform for analyzing in-line data for resistance spot welding quality monitoring and control.

Pacific Northwest National Laboratory and Oak Ridge National Laboratory

Inline weld quality monitoring is of paramount importance in manufacturing processes, particularly in automotive manufacturing where weld integrity directly impacts product performance, safety, and reliability. Among the car components, automotive battery trays play a critical role in housing and securing the vehicle's power source. The welds in these trays, particularly steel-steel welds, demand meticulous attention to detail to guarantee structural integrity and longevity. To address this challenge, the integration of machine learning (ML) techniques in automated weld quality monitoring and control emerges as a transformative solution, promising enhanced efficiency, accuracy, and consistency in production processes.

The research team has developed an expansible, interpretable ML platform that can monitor weld quality in real time. The platform is designed using resistance spot welding (RSW) process, weld structure/attribute and performance data provided by a U.S.-based original equipment manufacturer (OEM). The ML platform, featuring models developed by both the laboratories, is designed to seamlessly adapt to different materials, including advanced high strength steels and aluminum alloys. Its flexible architecture allows for the incorporation of diverse data sources and features, including images, categorical descriptors, as well as numerical inputs and enables accurate prediction across a wide range of materials.

Through the analysis of in-line process signals and postprocessed RSW joint data, ML models in the platform can detect deviations from optimal quality standards, by identifying signature data patterns and anomalies from inline signals and constructing the complex correlations with weld quality parameters. The platform incorporates physicsbased understanding of the correlations developed by integrating trust metrics in the analysis. The models, comprising of transparent Random Forests, XGBoost and support vector machines as well as deep learning methods in the ML platform have demonstrated greater than 98% accuracy in predicting whether a weld would meet the minimum weld nugget size requirement over a wide range of steel stack-ups, thickness, and welding conditions. Use of this platform will reduce the R&D time and resources for designing new stack-ups such as those geared towards lightweight joints by incorporating low density alloys and thinner plates. Moreover, the embedded continuous learning capabilities empower the ML tool to adapt and improve over time, optimizing weld quality assurance protocols.



Figure 1. Integrated expansible machine learning framework for weld process development and inline weld quality monitoring.

2023 U.S. DRIVE Highlight Solid Phase Processing of Aluminum Castings

Enabling thin-walled high pressure die cast aluminum alloys for structural use to achieve vehicle lightweighting and ease of assembly.

Pacific Northwest National Laboratory

Die casting is a reliable manufacturing method to fabricate near net shape parts in a fast and costeffective manner. Specifically, high pressure die cast (HPDC) aluminum alloy components provide great opportunity for vehicle lightweighting. However, to perform as a car body structural component, HPDC aluminum castings require an adequate combination of strength, ductility, and fatigue life. General-purpose HPDC aluminum alloys contain cast microstructure, needle-like silicon particles, and brittle second phase particles that negatively impact the strength and ductility, limiting their acceptance as structural car-body components.

Pacific Researchers at Northwest National Laboratory (PNNL) investigated effectiveness of friction stir processing (FSP), an innovative thermomechanical processing (TMP) method to improve strength and ductility of HPDC aluminum alloys. FSP can change the internal structure of a cast component into a dense and refined form. Since FSP can modify the internal structure of a casting at areas of interest, users can target select areas of a large casting for mechanical property enhancement. However, developing FSP methods for HPDC aluminum castings remain challenging because of limited wall thickness, high degree of casting porosity etc. There are added concerns about destroying the "good" mechanical properties of dieskin area by FSP method.

Researchers at PNNL came up with an optimized FSP tool design and processing methodology to improve the mechanical properties of two different HPDC aluminum alloys, (i) high-iron containing A380, and (ii) low-iron containing Aural-5. Research at PNNL demonstrated that FSP is able to generate a porosity-free wrought microstructure with the refinement of detrimental phases. A simultaneous

increase in strength and ductility led to better fatigue performance and fracture toughness, enabling better crashworthiness. Implementation of FSP on complex-shaped cast parts could be achieved using an industrial robotic platform.

Production of single piece ultra large HPDC aluminum alloy castings is the recent trend within automotive industry. Ultra large castings will help in part unitizing, reduce assembly time. FSP can enhance mechanical properties of ultra large castings at areas of interest, which can help in minimizing casting wall thickness to support vehicle lightweighting.



Figure 1. (a) FSP carried on a complex 3D profiled HPDC aluminum casting using robot. (b) Porosity inside casting. (c) FSP creates porosity-free internal structure. (d) Better fatigue properties after FSP. (e) Improved toughness after FSP.

Vehicle and Mobility System Analysis

2023 U.S. DRIVE Highlight

Vehicle Automation Impact on Mobility and Energy

This study quantified the impact of Adaptive Cruise Control and Coordinated Adaptive Cruise Control when deployed at scale across a wide range of metrics, including mobility, energy, emission and greenhouse gases.

Argonne National Laboratory

We studied the impact of various automated driving technology deployments on mobility, energy and emissions using the POLARIS-centered SMART Mobility workflow, developed under the U.S. Department of Energy's Energy Efficient Mobility Systems program. Extending previous work from 2022, we assessed the potential influence of multiple vehicle automation technologies. The mobility system model allowed us to study potential consequences such as changes in Vehicle Miles Travelled (VMT) and network speed, as well as impact on energy consumption and regional emissions.

All results were obtained from a simulation of the Austin metro area from 2015 to 2040 with population growth, evolving vehicle fleet and technology penetration varying from 1% to 90% deployment of:

- Adaptive Cruise Control (ACC)
- Level 2 Cooperative Adaptive Cruises Control (CACC)
- Level 4 Automated Driving with CACC

Both ACC and CACC were only deployed on the highway.

Key Findings:

- 11. Baseline congestion increases over time with 5% lower network speeds. ACC provides little to no benefit over time, while Level 2 CACC can improve network speeds. However, Level 4 CACC reduces it because of lower travel time cost and increased regional travel (Figure 1).
- 12. U.S. DRIVE program success (High Tech) for advanced vehicles simulated over time shows an increase in MPGGe by up to 20% by 2040 (Figure 2). Benefits of L4 vs L2 CACC appear to

counteract owing to increased L4 vehicle usage for travel. (Figure 2).

13. While advanced vehicle technologies lead to generally lower emissions (of up to 16% reduction), use of L4 CACC at 90% penetration by 2040 appears to lead potentially as much emissions as a baseline with Low tech. (Figure 2).









INFRASTRUCTURE AND INTEGRATION

Grid Integration



2023 U.S. DRIVE Highlight Cerberus: A Cyber-physical Security Mitigation Solution for High-Power EV Charging Infrastructure

Detection, response, and recovery from operational anomalies, and cyber or cyber-physical malicious exploits to ensure continued safe and resilient operation of high-power EV charging infrastructure.

Vehicle Technologies Office

Cybersecurity and cyber-physical security of highpower charging infrastructure for electric vehicles (EVs) is critical to safety, reliability, and consumer confidence in this publicly accessible technology. At Laboratory Idaho National (INL), several cybersecurity and cyber-physical security best practices are incorporated into a proof-of-concept anomaly detection and mitigation solution known as Cerberus, designed after industrial Safety Instrumented Systems (SIS) to ensure robust and resilient operational safety.

Cerberus is intended to secure high-power DC chargers or extreme fast chargers (XFC) at a charge site from cyber and cyber-physical exploitation and other anomalous events. Cerberus is designed to detect anomalous behavior, respond accordingly based on the potential impact severity, and if possible, recover the system for continued safe charging of EVs.

Cerberus, as shown in Figure 1, is comprised of a core module integrated into each electric vehicle supply equipment (EVSE) and an aggregator module at each charge site. Each core module monitors EVSE communications with the EV, Open Charge Point Protocol (OCPP) server, and other external communications. Each core module also monitors the internal controls communication of the EVSE including the thermal management system, power electronics, safety systems, and graphical user interface. Cerberus integrates sensors in numerous sub-systems and redundantly verifies the AC and DC current, voltage, power quality, temperature, and the state of numerous sub-systems within the EVSE such as the door latch sensors. Upon detection of an anomalous state or event, the core module takes appropriate mitigation action based on the potential impact severity. Additionally, the core module broadcasts a descriptive message through a Secure

Shell (SSH) tunnel of the anomalous event in the form of a warning, alert, or error code to the Cerberus aggregator, a coordination module that receives information from each core module and takes site-wide action in response to widespread exploits or events. The aggregator can determine the extent of a malicious or anomalous event by analyzing the combined information from the core modules. This is effective for events that may seem rather benign at each core module but together with similar anomalous characteristics are determined to be caused by a widespread event.



INL initially conceptualized and proved Cerberus as a valid concept in the Vehicle Technologies Officefunded *Consequence-driven Cybersecurity for High-Power EV Charging Infrastructure* ("3C") project in FY19-FY21. The Cerberus system was improved upon and augmented with additional response and recovery capabilities for cybersecurity and resiliency in the EVs@Scale Consortium cyberphysical security pillar in FY22-FY23. Cerberus was also a cornerstone of DOE's CESER office-funded *Electric Vehicle Secure Architecture Laboratory Demonstration* (EV SALaD) of cybersecurity best practices for high-power charging infrastructure. Cerberus was a winner of the 2023 R&D 100 award.



2023 U.S. DRIVE Highlight Roadmap of Standards and Codes for Electric Vehicles at Scale (EVs@Scale)

A DOE/American National Standards Institute (ANSI) initiative to identify and address the challenges of charging electric vehicles at scale (EVs@Scale), the grid, and standards and codes.

Vehicle Technologies Office

With millions of electric vehicles (EVs) now on American roads and the rapid evolution of EV and charging technologies, the development and harmonization of standards and codes for EV-grid integration is of paramount importance. The focus of this **roadmap** is to identify standards, codes, and conformance programs needed to facilitate the safe, mass deployment of EVs and charging infrastructure in the U.S. with international coordination, adaptability, and engagement. The roadmap also identifies existing issues, guides, and related policies and those that are currently in development. It identifies gaps and recommends development of new or revised standards, specifications, and conformance and training programs, where needed. The roadmap's primary focus is light-duty, on-road plug-in EVs that are recharged via connection with the electrical grid, as well as the supporting charging infrastructure. The roadmap also considers medium- and heavyduty EVs, as well as wireless charging. The target audience includes vehicle manufacturers; entities that will be installing and operating standards development infrastructure: organizations (SDOs); U.S. federal, state, and municipal agencies; electric utilities; and others.

The roadmap identifies a total of 37 gaps with corresponding recommendations across the topical areas of vehicle systems, charging infrastructure, grid integration, and cybersecurity. A gap implies that no published standard, code, regulation, or policy exists that sufficiently covers the issue at hand. Of the 37 gaps, the roadmap identifies 14 gaps/recommendations as high priority, 20 as medium priority, and 3 as low priority. In 23 cases, additional pre-standardization research and development (R&D) is needed. The roadmap also suggests priorities, timeframes for standards development, and organizations that may be able to develop the standards or perform supporting R&D. The roadmap targets the U.S. market with international harmonization issues emphasized in key areas. Approximately 130 individuals from 80 public- and private-sector organizations supported the document's development, including U.S. federal government agencies and national laboratories, SDOs, industry, academia, and others. The roadmap development process was open to all EV stakeholders with operations in the U.S.

	High Priority (0-2 years)	Medium Priority (2-5 years)	Low Priority (5+ years)	Total
Vehicle Systems	5	1	0	6
Charging Infrastructure	2	4	2	8
Grid Integration	3	11	1	15
Cybersecurity	4	4	0	8
Total	14	20*	3*	37

*(23 gaps require pre-standardization R&D)

Figure 1. Breakdown of Gaps for Standards and Codes

Next Steps: VTO and ANSI will establish mechanisms to assess progress in implementing the roadmap's recommendations. A priority is increasing awareness about roadmap availability and recommendations, especially to organizations identified as instrumental to resolution of gaps. Ultimately, strong collaboration and coordination among stakeholders are essential to close the identified gaps and advance EV-grid integration.

2023 U.S. DRIVE Highlight Next-Gen Profiles Project

A U.S. DOE EVs@Scale Consortium multi-national laboratory project conducted to characterize, assess, and mitigate the impacts of High-Power electric vehicle charging on the grid infrastructure.

Vehicle Technologies Office EVs@Scale National Lab Consortium

To characterize the diversity of charging profiles and performance between electric vehicles (EVs) and electric vehicle supply equipment (EVSE) utilizing High Power Charging, as well as identify grid impacts, the Vehicle Technologies Office (VTO) is conducting the Next-Gen Profiles (NGP) project as a multi-laboratory effort separated into three categories: EV Profile Capture, EVSE Characterization, and Fleet Utilization. The project aims to capture and analyze the charging profiles and behaviors across a wide variety of boundary conditions.

EV Profile Capture characterizes the charging profiles of EVs and EVSE using measurable parameters. In 2023, 164 profiles across 13 EVs were captured. Figure 1 is an example of EV profile data.



EVSE Characterization captures quasi-steady state performance characteristics of the EVSE system across a wide range of conditions, such as voltage and current operating range and harmonics. In 2023, both conductive and non-conductive EVSE systems were characterized.

Fleet Utilization characterizes the behavioral utilization of real-world fleets utilizing HPC EVs and EVSE. In 2023, one EV fleet and three EVSE were analyzed. Figure 2 is an example of fleet data.



Figure 2. Average weekly utilization of the metric Total Charge Time (min), averaged over each hour of the week for the entire dataset.

The research performed in these three areas of interest by Argonne National Laboratory, Idaho National Laboratory, National Renewable Energy Laboratory, and Oak Ridge National Laboratory yielded four Energy Efficiency and Renewable Energy technical reports posted to DOE's Office of Scientific and Technical Information website.

- 1. High Level Analysis 2023.docx
- 2. EV Profile Capture 2023.docx
- 3. EVSE Characterization 2023.docx
- 4. <u>Fleet Utilization 2023.docx</u>

Throughout 2023, the NGP team gave presentations at EVs@Scale deep dives and semi-annual meetings to keep industry and shareholders updated on our team's progress.

In 2024 the NGP team has begun a project procedures revision to include recent scope additions that will gather industry input and feedback. Integration of EV charge profiles into grid modeling platforms is underway. Additional EV and EVSE assets have been gathered for this year's data capture, and multiple fleets have been added. An updated, new set of technical reports is scheduled to be completed end of CY2024.

(This Page Intentionally Left Blank)