CERC-CVC: U.S. - China Clean Energy Research Center Clean Vehicles Consortium

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A consortium lead by

The University of Michigan and Tsinghua University

in partnership with

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Executive Summary

Project Management Highlights

Project Scope

Over the last quarter, CERC-CVC has continued to focus on key areas of interest to our industrial partners, and CERC-CVC has also started looking at what research topics might be covered in a possible 2nd phase of CERC-CVC. To that end, the 4th CERC Steering Committee meeting was held in Beijing on July 11th. The meeting was chaired by Secretary Ernest Moniz (US DOE) and Minister WAN Gang (China MOST). Other attendees included the US Ambassador to China Mr. Max Baucus and Director of the US Trade and Development Agency Ms. Leocadia Zak. Dr. Andy Brown (Delphi) and Dr. Wei Shen (Ford) attended the meeting as the US IAB representatives for CERC-CVC.

After getting a thorough overview of the CERC research, Secretary Moniz and Minister WAN had the following feedback:

- The overall CERC program should continue, and should be strengthened.
- Each CERC center should operate with a 10-year view even though only 5-years funding was initially provided. If a second phase is funded, the scope should be further refined by developing a roadmap of how to achieve the desired outcomes.
- It is even more important to leverage the limited government resource in the 2nd phase.
- There should be more discussion on standards to support implementation of new technologies.
- IP protection remains critical for the CERC program.

Overall, Secretary Moniz mentioned a possible 2nd phase of CERC multiple times and he was supportive of the proposed CERC-CVC research themes presented at the meeting. To that end, we have been tasked with developing CERC 2.0 proposals for his consideration and discussion with Minister Wan in September. The proposals will include roadmaps with milestones and clear paths to public benefits (for both countries), and will be aligned more closely with DOE's VTP program objectives.

Collaboration

- CERC Steering Committee meeting, June 11th, Beijing, China
- Upcoming CERC-CVC annual meeting, August 11th and 12th
- Monthly Thrust Area Web Ex meetings are running regularly and have been scheduled midway through 2014

Project Overview

Thrust Area	Project ID	Project Name	Research Lead	Collaboration Status
Thrust 1: Advanced Batteries				
1	1	Characterization of Degradation Mechanisms in Li-Ion Batteries	OSU/SNL /ORNL	Joint
1	2	High Energy Density Battery Chemistries	UM/MIT	Joint
1	3	Modeling and Control of Lithium-Ion Batteries	THU	Cooperative (China)
Thrust 2: Clean Combustion and Energy Conversion				
2	1	Advanced Biofuels	SNL/UM/ ORNL/ THU	Joint
2	2	Integrated powertrain and aftertreatment system control for clean vehicles	OSU/THU /SJTU	Joint
2	3	Auxiliary Power Unit	SJTU /THU	Cooperative (China)
2	4	Energy Conversion	UM/OSU/ WUT	Joint
Thrust 3: Vehicle Electrification				
3	1	Efficient and high-power density electric powertrain	UM	Joint
3	2	Control and optimization of distributed vehicle network	THU	Cooperative (China)
3	3	System integration technologies for improved efficiency, safety, reliability and NVH performance	OSU/UM	Joint
3	4	Battery Modeling and Control	UM	Joint
Thrust 4: Advanced Lightweight Materials and Structures				
4	1	Forming processes for lightweight materials	SJTU	Joint
4	2	Cost effective lightweight materials	OSU	Cooperative (US)
4	3	Joining in Multi-Material Vehicle Structures	OSU/UM	Joint
4	4	Multi-Material Lightweight body subsystem & vehicle optimization	UM	Joint
Thrust 5: Vehicle Grid Interface				
5	1	System architecture and interaction mechanism of ITS based V2G	TSU/ OSU	Joint
5	2	Vehicle-Grid System modeling for technology deployment	OSU/ TSU	Joint
5	3	Control strategies for vehicle-grid integration	UM	Joint
5	4	A Wireless Magnetic-Resonance Power Transmission System for EV Charging	UM	Cooperative (US)

Thrust Area	Project ID	Project Name	Research Lead	Collaboration Status
Thrust 6: Energy Systems Analysis, Technology Roadmaps and Policy				
6	1	Set CV Technology energy efficiency and GHG Targets and Evaluate Life cycle Performance	UM	Joint
6	2	Fuel Mix Strategies and Constraints	SNL/UM	Cooperative (US)
6	3	Fuel economy and GHG standards and labels for PEVs from a life cycle perspective	UM	Joint
6	4	CV Technology Roadmap and Policy Recommendations	MIT/UM	Cooperative (US)
6	5	Electricity and material sourcing scenario analyses to guide vehicle technology strategies	UM	Cooperative (US)
			Cooperative (US)	**5**
			Joint	**16**
			Cooperative (China)	**3**

Cost Status

DOE has now fully funded CERC-CVC with $2.5M annual funding in Period 3 as well as $1.2M for Period 4. Period 4 now encompasses the remaining time on the contract, and the total cost-share spending reflects the figure in the original proposal as submitted through the end of the award. While total Authorized Federal Funds total approximately $8.5M, current cash receipts are lagging behind at approximately $7M. With expenditures topping $7.2M, we are now operating at a cash deficit until the next tranche of funds is received from the Department of Energy.

Budget Period 1 - 4	Budgeted	Actual
DOE	$ 8,515,180	$ 7,210,775
Cost-share	$ 17,012,837	$ 7,979,558
Total	$25,528,017	$15,190,333

Schedule Status

Work continues on schedule as outlined in the Joint Work Plan with a 6 month shift of timing due to the delays in contracting.

Publications / Key Outcomes / Awards

Advanced Batteries and Energy Conversion

D. E. Demirocak, B Bhushan. "In-situ atomic force microscopy analysis of morphology and particle size changes in LiFePO4 cathode", *Journal of Colloid and Interface Science*, 423, 151-7 (2014)

Danny X. Liu, Jinghui Wang, Pan Ke, Jie Qiu, Marcello Canova, Lei. R. Cao and Anne C. Co, "In Situ Quantification and Visualization of Lithium Transport with Neutrons," *accepted by Angewandte Chemie International Edition.*

Delivered two invited presentations that acknowledge CERC funding:

1. 1st International Symposium on Sustainable Secondary Battery Manufacturing and Recycling, June 29-July 4, 2014, Cancun, Mexico
2. U.S. Nat. Congress on Theoretical and Applied Mechanics, June 15-20, 2014, East Lansing, MI

Two posters presented at Beyond Lithium Ion 7 Conference that acknowledge CERC funding:

1. Nitin Kumar, Maxwell D. Radin, D. J. Siegel, "DME Decomposition on Li2O2 Surfaces: Peroxide vs. Superoxide Terminations," Beyond Lithium Ion VII, Argonne, Illinois, June 3-5 2014

Sheng Yang and D. J. Siegel "Charge transport in Na-O2 batteries," Beyond Lithium Ion VII, Argonne, Illinois, June 3-5 2014

Kwabi, D.G., Batcho, T.P., Amanchukwu, C.V., Ortiz-Vitoriano, N., Hammond, P., Thompson, C.V., Shao-Horn, Y. (2014). "Chemical Stability of dimethyl sulfoxide in lithium-air batteries" *Submitted for publication*

Advanced Biofuels, Clean Combustion and Auxiliary Power Unit (APU)

Ab Initio Investigation of the Thermal Decomposition of n-Butylcyclohexane. Mohamad Akbar Ali, V. Tyler Dillstrom, Jason Y. W. Lai and Angela Violi *The Journal of Physical Chemistry A* 118 pp. 1067-1076 (2014)

Pingen Chen, Umar Ibrahim, and Junmin Wang, "Experimental Investigation of Diesel and Biodiesel Post Injections during Active Diesel Particulate Filter Regenerations," *Fuel*, Vol. 130, pp. 286 - 295, 2014.

Junfeng Zhao and Junmin Wang, "Model Predictive Control of Integrated Hybrid Electric Powertrains Coupled with Aftertreatment Systems" *Proceedings of the 2014 ASME Dynamic Systems and Control Conference*, 2014 (accepted).

W. Liu, H. Chi, H. Sun, Q. Zhang, K. Yin, X. F. Tang, Q. Zhang, and C. Uher, "Advanced Thermoelectrics Governed by Single Parabolic Band: $Mg_2Si_{0.3}Sn_{0.7}$, a Canonical Example", *Phys. Chem. Chem. Phys*. **16**, 6893-6897 (2014).

X. F. Tang, X. Su, F. Fu, Y. Yan, and C. Uher, "Combustion Synthesis Applied to Compound Thermoelectric Semiconductors: a New Criterion for Applicability of Combustion Processing", an invited talk at the International Conference on Thermoelectrics, Nashville, July 8, 2014.

S. Hui, J. R. Salvador, K. P. Pipe, and C. Uher, "Effect of Sn Dopants on the Thermoelectric Properties of p-type Yb-filled Skutterudites", an oral presentation at the International Conference on Thermoelectrics, Nashville, July 9, 2014.

M. J. Adams, M. D. Nielsen, and J. P. Heremans, "Improving Electronic Properties of Al-doped CoSb3", an oral presentation at the International Conference on Thermoelectrics, Nashville, July 9, 2014.

Vehicle Electrification

"Steady-State Algorithms for Nonlinear Time-Periodic Magnetic Diffusion Problems using Diagonally-Implicit Runge-Kutta Methods" has been accepted for publication, pending revisions, by IEEE Transactions on Magnetics.

Journal Paper Accepted: Xiaowu Zhang, Huei Peng, Jing Sun, "*A Near-Optimal Power Management Strategy for Rapid Component Sizing of Multi-mode Power Split Hybrid Vehicles*", IEEE Transactions of Control System Technology

Conference Paper Accepted: Xiaowu Zhang, Huei Peng, Jing Sun, "*Automated Modeling and Mode Screening for Exhaustive Search of Double-Planetary-Gear Power Split Hybrid Powertrains*", 2014 Dynamic System and Control Conference, Santino, TX

Jiyu Zhang, Giorgio Rizzoni, "*Structural Analysis for FDI of PMSM Drive System in Electric Vehicles*". *To be presented at ITEC Asia 2014*

Zhou, X., Ersal, T., Stein, J. L., and Bernstein, D. S., 2014. "*Battery State of Health Monitoring by Side Reaction Current Density Estimation via Retrospective-Cost Subsystem Identification*". ASME Annual Dynamic Systems and Control Conference, accepted.

Advanced Lightweight Materials and Structures

Ziwei Zhao, Wei-Ching Liao, L. James Lee, Jose M. Castro. "*Permeability analysis of carbon nanofiber nanopapers*." 30th International Conference of the Polymer Processing Society, 2014.

Wei-Ching Liao, Eusebio D. Cabrera, Ziwei Zhao, Ying-Chieh Yen, Jiangfeng Yu, Jose M. Castro, L. James, Lee. "*Simulation of nanopaper permeability and injection molding using smoothed particle hydrodynamics*." 30th International Conference of the Polymer Processing Society, 2014.

A. Vivek, S.R. Hansen, and G.S. Daehn, "High strain rate metalworking with vaporizing foil actuator: Control of flyer velocity by varying input energy and foil thickness," *Review of Scientific Instruments*, **85**, 075101-1, 8 (2014).

S.R. Hansen, A. Vivek, and G.S. Daehn, "Control of Velocity, Driving Pressure, and Planarity in Flyer Launch with Vaporizing Foil Actuator," submitted to 6th International Conference on High Speed Forming, Daejon Korea, April 2014.

Patent 2115-005675-US-PS1, Hybrid Friction Stir Welding for Dissimilar Materials Through Electro-Plastic Effect, Xun Liu, Shuhuai Lan, Jun Ni, referenced provisional patent application filed

Vehicle-Grid Integration

C. Weiller and R. Sioshansi, "*The Role of Plug-In Electric Vehicles with Renewable Resources in Electricity Systems*," submitted to *Revue d'Économie Industrielle*

"Coordinated PEV Charging and its Effect on Distribution Network," to be presented at the Power Systems Computation Conference in Wroclaw, Poland August 18-22, 2014

A Wireless Magnetic-Resonance Power Transmission System for EV Charging

- Presented one paper at the IEEE APEC March 2014;
- One paper accepted by IEEE Transactions on Vehicular Technology
- One paper accepted by IEEE Journal of Emerging and Selected Topics in Power Electronics, Special Issue on Wireless Power Transfer
- Filed three patent in US and two patents in China; world patent rights are planned

Energy Systems Analysis, Technology Roadmaps and Policy

Lewis, A.M., J.C. Kelly, G.A. Keoleian. Vehicle lightweighting vs. electrification: Life cycle energy and GHG emissions results for diverse powertrain vehicles. *Applied Energy* (2014) 126: 13–20.

Lewis, A., Keoleian, G., and Kelly, J., "The Potential of Lightweight Materials and Advanced Combustion Engines to Reduce Life Cycle Energy and Greenhouse Gas Emissions," *SAE Technical Paper* 2014-01-1963, 2014, doi:10.4271/2014-01-1963.

"The Impact of the Grid on Vehicle Life Cycle Sustainability" Steel Market Development Institute, Livonia, MI, May 14, 2014. (Presentation)

"Reducing GHG Emissions from Vehicle Lightweighting and Electrification? The power of the grid." Emissions 2014, Global Automotive Management Council Conference, June 11, 2014. (Presentation)

Informing Electric Vehicle Public Charging Infrastructure Development using Travel Patterns Mined from Big-Data" awarded 3rd Place Student Paper in 2014 International Symposium on Sustainable Systems and Technology (ISSST) held in Oakland, California.

"The liquid carbon challenge: evolving views on transportation fuels and climate" by J.M. DeCicco in *WIREs Energy & Environment*; the online preprint was posted 8 July 2014. doi:10.1002/wene.133

Technical Progress Summary

Research and development in the clean energy sectors in the U.S. and China, the world's largest energy producers, energy consumers and greenhouse gas emitters, is an important area of opportunity for both countries. Developing and deploying clean transportation technologies in the world's two largest automobile markets and oil consumers is a key contributor towards meeting energy and climate challenges in the years ahead. To achieve clean transportation solutions, the CERC-CVC has collaboratively grown basic research knowledge and technology development since its inception to achieve the solutions necessary to reduce the dependence of vehicles on oil and improve vehicle fuel efficiency.

The CERC CVC has focused on maximizing collaborative efforts and leveraging the respective strengths of the research partners to accelerate invention and commercial success in a range of focus areas: advanced batteries and energy conversion; advanced biofuels and clean combustion; vehicle electrification; advanced lightweight materials and structures; vehicle-grid interactions; and energy systems analysis, technology roadmaps and policies. The team, consisting of academic institutions in the U.S. and China, U.S. national laboratories, and strategic partners from industry is making steady progress with basic science discovery, technology development, and U.S. China collaborative scientific activities.

In the advanced battery systems thrust, work continues to reveal possible degradation mechanisms in Li-Ion batteries. While chemical degradation mechanisms have been studied extensively, mechanical degradation mechanisms have received little attention so far. We are using nano-indentation to probe the nano-mechanical properties (i.e., elasticity of modulus and hardness) of a thin film $LiFePO_4$ cathode by comparing un-aged and aged cathodes. This research will lead to an enhanced understanding of the mechanical properties of the un-aged and aged thin film cathode and the mechanical degradation mechanisms in Li-ion batteries. A new subtask was initiated to further support the thrust focused on manufacturing pouch cells for battery degradation studies. The Battery Manufacturing Facility at Oak Ridge National Laboratory is producing pouch sells ranging from 100 mAH to 7 Ah for either characterization studies or degradation studies.

In the biofuels and APU thrust, important fundamental work continues to model novel biofuel molecules. To date, seven molecules have been studied that constitute the key components of structurally complex biofuels produced using microbial synthesis. Key features related to their low-temperature ignition characteristics are being studied. In this quarter, the laser-absorption measurements of OH and HO_2 time histories were completed for 2,5-dimethylhexane, a key component of bisabolene. Powertrain efficiency gains post engine in the area of thermo electrics focused on studying transport measurements of newly fabricated Sn-filled and Sn-doped p-type $Yb_xFe_4Sb_{12}$ skutterudites samples.

In the electrification thrust, the MATLAB toolbox developed for electric machines is being revised to allow for more flexibility in the investigation of different winding structures, source

types, and external circuits. The toolbox update will allow straightforward modeling of the asynchronous machine rotor topology. The developed codes are also being used in two industry funded projects, one to design an electric machine for an EV traction drive and one to validate performance of an electric machine. Moving to the full-scale powertrain design, the systematic design procedure has been deployed to search the design space of double planetary gear systems with all possible clutch locations. Based on input from Ford, drivability was considered as the primary screening criterion, and a new methodology was developed to analyze drivability. Researchers are closely collaborating with Ford with the aim to develop a power-split hybrid design for the F-150 truck. The adaptive battery management system team has focused on the design of an experimental setup for battery module testing which would allow for application of the previously developed incremental capacity analysis based lithium ion battery state of health monitoring.

In the area of lightweight materials, the development of cost-effective lightweight structures, joining processes and vehicle subsystem optimization continues. New cost effective composites must balance performance with processablility. In the area of joining multi-material structures, we are now investigating longer continuous sheet-to-sheet solid-state welds using a newly built vaporizing foil actuator metalworking fixture, which is capable of handling workpieces with an active working region of up to 9 inches. The friction stir welding research has focused on investigating the thermal effects due to resistance heating. The temperature was measured during the stir welding process by burying three thermocouples along the weldline in the backing plate. In the multi-material lightweight body systems task, research focus has shifted to improving computational cost of sampling the design space and parallelization to further save data generation time.

Electrification is not just promising for increased efficiency; it also allows vehicles to interface with the electric grid and possibly renewable energy sources. In the area of systems modeling, the effects of level-3 fast PEV charging stations co-located with big-box retailers on aging of existing transformers has been modeled, and work is underway to develop the structure for stochastic dynamic programming model to use distributed generation and energy storage to relieve transformer loading due to level-3 fast PEV charging. This work is synergistic with the development of a wireless magnetic-resonance power transmission system. Work is underway to develop, design, and test a hardware prototype for placement in an automotive environment to test the performance.

Finally, work continues in thrust area 6, the energy systems analysis, technology roadmaps, and policy thrust. The vehicle design and assessment work is refining the life cycle inventory of the material and manufacturing processes for a wireless charger based on a tear down of a sample charger provided by Delphi. With respect to alternative fuel vehicle fleet analysis, analyses were completed that consider impact of range penalties, infrastructure availability, and recharge time on BEV adoption using driving distributions that represent real world data. In addition, researchers have projected the growth, energy consumption, and CO_2 emissions of electrified vehicles, including BEV, HEV and PHEV in China for the next 35 years and forecasted the electric utility capacity expansion and the energy mix in China for the next 35 years. They also

predicted the amount of CO_2 emissions and air pollution that can be reduced through the penetration of electrified vehicles, and map whether emissions would be distributed to rural areas instead.

What follows outlines in more details the accomplishments of the CERC-CVC to date. Each project has outlined the current progress towards the stated research objectives, and highlighted collaboration with their Chinese counterparts, and industry members of the CERC-CVC. The work has already resulted in a number of scientific publications, and the further intellectual property disclosures are being made.

Detailed Project Reporting

Thrust Area 1: Advanced Batteries

Thrust	TA1: Advanced Batteries and Energy Conversion
Title	**Project 1.1.: Characterization of Degradation Mechanisms in Li-Ion Batteries**
Personnel	PIs: Bharat Bhushan (OSU), Marcello Canova (OSU), Lei (Raymond) Cao (OSU), David McComb (OSU) PDR: Dervis Emre Demirocak (OSU), Shrikant C. Nagpure (OSU) GRA: Samartha Channagiri (OSU), Sanjay Ramdon (OSU),
Objective	The objective of this project is to characterize the aging mechanisms of $LiFePO_4$ batteries on different scales and through varying techniques.
Progress Report	1. Aging Cells: Aging of an 8 cell batch of A123 20Ah prismatic cells is currently in progress. The aging protocol being followed is a charge depletion mode defined by the USABC for hybrid electric vehicles. 2. In-situ Electrochemical AFM: This work has been completed and the results published (see notable achievements section) 3. Nano-mechanical Characterization: This task has been completed. Results are presented in the paper titled, "Nanomechanical Characterization and Mechanical Integrity of Unaged and Aged Li-Ion Battery Cathodes," accepted for publication in Journal of Power Sources (see notable achievements section). 4. X-ray Micro-computed Tomography Analysis for Characterizing Porosity: This task has been completed. A research paper based on the results of this has been published in "The Journal of Power Sources" (listed in notable achievements section). 5. X-Ray diffraction: This task has been completed. The results were used to further analyze the results of the tomography study. They are included in the above-mentioned publication. 6. Electron Energy Loss Spectroscopy (EELS) for the Study of Local Bonding Within Cathode Material: Cathode material was harvested from an unaged and aged sample of an A123® 20Ah prismatic $LiFePO_4$ cell. The aged sample was aged at 55 C until 90 percent capacity retention using a charge depletion profile defined by the USABC. Focused ion beam milling was used to extract electron transparent thin foils (Fig.1) from the harvested cathodes from both cells for EELS analysis. EELS has been performed on a standard nanoparticle (Fig.2), unaged and aged battery samples using a Tecnai TF 20 microscope operating in STEM mode. The high tension used was 200kV, energy resolution ~ 1eV and a dispersion = 0.1eV /channel. These parameters allowed us to collect valence and core loss data (including Li-K and Fe-M twin peaks) (Fig.2). The height and position of the Li-K / Fe-M twin peak can be used to judge the amount of Lithium, oxidation state of iron and the nature of bonding around iron. Data from the standard particle, unaged and aged cells is currently being analyzed. 7. In-situ X-Ray Diffraction and Scanning Transmission X-ray Microscopy: As suggested last time, a second in-situ cell was designed and tested. We were unable to observe any $LiFePO_4$/$FePO_4$ peaks in the reflection mode XRD pattern of the coin cell with the working electrode facing upwards.

This is most likely due to the unavoidable, thick aluminum layer on top (~10µm) and sample alignment limitations. As a result, we have decided to perform in-situ XRD and STXM (Scanning Transmission X-ray Microscopy) in the synchrotron. The synchrotron source will help us tune source wavelength, while also providing a higher flux and option for focusing the source using zone plates, to high resolutions (~60nm). In-situ XRD will provide phase information averaged over a large area (a few millimeters), while in-situ STXM will provide spatial phase distribution information within the cathode. A split cell has been designed based on existing designs in literature and necessary arrangements are being made for using the right beamline for the chosen experiments

8. Standards Analysis: Standards for XRD have to be re-performed in the synchrotron based on the experimental conditions chosen for the in-situ experiment, which are yet to be decided.

9. In situ atomic force microscopy analysis of morphology and particle size changes in Lithium Iron Phosphate cathode during discharge: The results of this work mentioned in the last report have been published and the reference provided below in the notable achievements section [4].

10. Probing the aging effects on nanomechanical properties of thin film $LiFePO_4$ Li-ion batteries: Thin film Li-ion batteries are considered to have great potential in many small scale electronic devices such as medical implants, microchips and microelectromechanical systems (MEMS), where space to accommodate a battery is very limited and capacity and power requirements are not very high. In addition, thin film Li-ion batteries can be utilized in flexible electronics as well as they can be integrated into electronics in a bottom-up approach to save space and weight. Apart from the application point of view, thin film battery cathodes are also more suitable for fundamental research since they only include active material (i.e., $LiFePO_4$) as opposed to composite battery cathodes (i.e., regular battery cathodes) which include carbon coated $LiFePO_4$ active material dispersed in PVDF binder.

    One of the challenges is to improve the cycle life of Li-ion batteries which requires detailed understanding of the aging phenomenon. The aging mechanism of Li-ion batteries can have both chemical and mechanical origins depending on the Li-ion battery subcomponents (i.e., cathode, anode, separator and current collector). While the chemical degradation mechanisms have been studied extensively, mechanical degradation mechanisms have received little attention so far.

    $LiFePO_4$ is one of the promising Li-ion chemistries among others due to its high theoretical capacity, superior cycle life, thermal stability and low cost. Mechanical properties of $LiFePO_4$ in de/-lithiated states have been studied theoretically, but experimental studies are rather scarce, and more importantly, concentrated on composite commercial battery cathodes. To the best of our knowledge nanomechanical properties of $LiFePO_4$ active material has not been reported so far. In this study, using nanoindentation we will probe the nanomechanical properties (i.e., elasticity of modulus and hardness) of a thin film $LiFePO_4$ cathode by comparing unaged and aged

	cathodes. Thin film $LiFePO_4$ cathode will be deposited on Ti, stainless steel or silicon substrates by physical vapor deposition (i.e., RF magnetron sputtering), (Fig. 3). Nanomechanical properties will be evaluated using the Hysitron nanoindenter. Structural and morphological properties of the thin film cathodes will be studied by XRD, AFM and SEM. The XRD spectrum of thin film $LiFePO_4$ is given in Fig.4. This research will lead to an enhanced understanding of the mechanical properties of the unaged and aged thin film $LiFePO_4$ cathode and the mechanical degradation mechanisms in Li-ion batteries.
Industry Collaboration	• None
US-China Collaboration Activities	• None
Issues of Concern	None
Notable Recent Achievements	1. S.A Channagiri, S.C. Nagpure, S.S. Babu, G.J. Noble, R.T. Hart "Porosity and Phase Fraction Evolution with Aging in Lithium Iron Phosphate Battery Cathodes", *J. Power Sources*, **243,** 750–757, (2013) 2. Ramdon, S., and Bhushan, B. "Nanomechanical Characterization and Mechanical Integrity of Unaged and Aged Li-ion Battery Cathodes," *J. Power Sources*, (accepted) 3. S. Ramdon, B. Bhushan and S. C. Nagpure, "In situ electrochemical studies of lithium-ion battery cathodes using atomic force microscopy", *J. Power Sources*, 249, 373–384 (2013) 4. D. E. Demirocak, B Bhushan. "In-situ atomic force microscopy analysis of morphology and particle size changes in LiFePO4 cathode", *Journal of Colloid and Interface Science*, 423, 151-7 (2014)

Appendix:

Articles Reviewed:

[1] Y. Orikasa, T. Maeda, Y. Koyama, T. Minato, H. Murayama, K. Fukuda, H. Tanida, H. Arai, E. Matsubara, Y. Uchimoto and Z. Ogumib, "Phase Transition Analysis between $LiFePO_4$ and $FePO_4$ by In-Situ Time-Resolved X-ray Absorption and X-ray Diffraction," *J. Electrochem. Soc.,* **160 (5),** A3061-A3065, (2013).

[2] A.S. Andersson, B. Kalska, L. Haggstrom, J.O. Thomas, "Lithium Extraction/Insertion in $LiFePO_4$: an X-Ray Diffraction and Mossbauer Spectroscopy Study," *Solid State Ionics,* **130,** 41-52, (2000)

[3] H-H. Chang, C-C. Chang, H-C Wub, M-H Yang, H-S Sheu, N-L Wua, "Study on Dynamics of Structural Transformation during Charge/Discharge of $LiFePO_4$ Cathode" *Electrochem. Comm.,* **10,** 335-339, (2008).

[4] M. A. Rodriguez, D. Ingersoll, and D. H. Doughty, "An Electrochemical Cell for In-situ Characterization" *Advance in X-Ray Analysis,* **42,** 267-275, (2000).

[5] Th. Koop , W. Schindler, A. Kazimirov, G. Scherb, J. Zegenhagen, Th. Schulz , R. Feidenhans, J. Kirschner, "Electrochemical Cell for In-situ X-ray Diffraction Under Ultrapure Conditions", *Rev. Sci. Inst.,* **69 (4),** 1840-1843, (1998).

[6] T. Nakamura, S. Masuda, Y. Yamada, H. Takahara, W. Yashiro, "In-situ X-ray Diffraction Study on $LiFePO_4$ Olivine Cathode" *220th ECS Meeting* (2011).

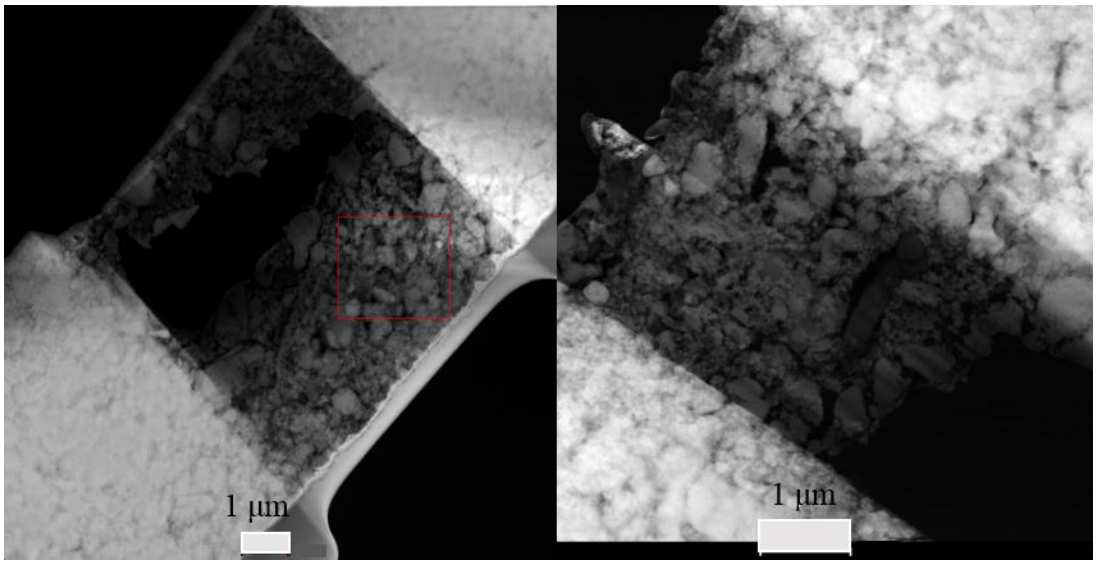


Fig. 1: FIB foils from an unaged (a) and aged (b) specimen

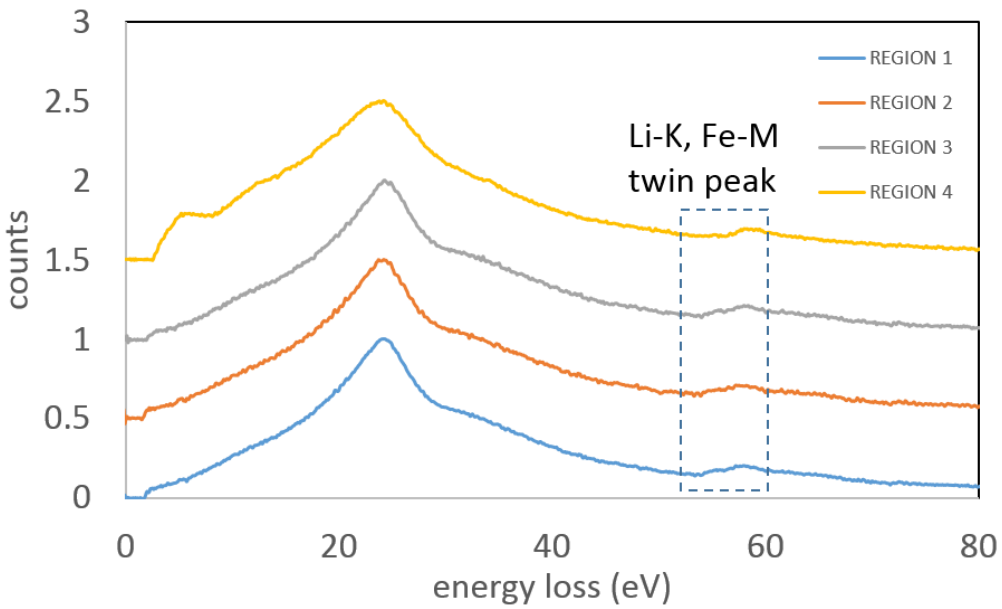


Fig.2: A comparison plot showing several EELS spectra from different regions within a nanoparticle of $LiFePO_4$ taken from a standard specimen showing the twin peak structure of Li-K / Fe-M

Fig. 3: Schematic of thin film $LiFePO_4$ synthesized by RF magnetron sputtering.

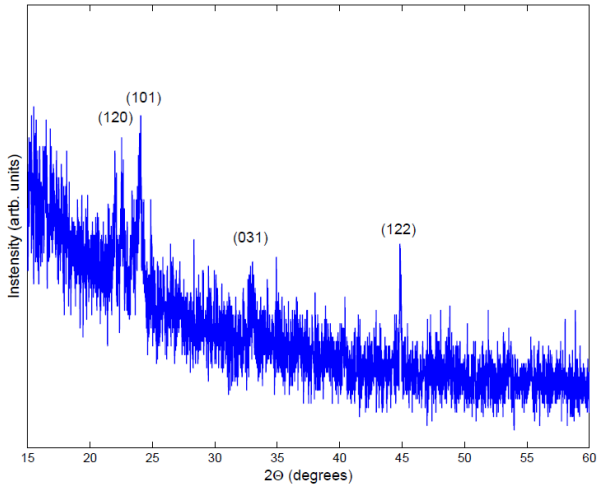


Fig. 4: XRD peaks of thin film $LiFePO_4$ deposited on Si substrate. Sample treated at 700°C for 2 h under 5%H_2/95%N_2 atmosphere.

Thrust	TA 1: Advanced Batteries and Energy Conversion
Title	**Project 1.2: In-situ Neutron Depth Profiling of Lithium Ion Battery Materials for Improved Electrochemical Performance and Aging Models (US Cooperative)**
Personnel	PIs: Marcello Canova (OSU), Raymond Cao (OSU), Anne Co (OSU) GRA: Danny Liu (OSU), Jinghui Wang (OSU)
Objective	• To establish a direct and non-destructive method for measure lithium transport in commercial lithium-ion battery anodes and cathodes; • To establish a technique for conducting in-situ measurement of the lithium concentration and distribution within the anode and cathode of lithium-ion cells during cell utilization (discharging and charging); • To identify the effect of aging, lithium distribution and transportation in anodes and cathodes through direct in-situ measurements. • To improve the accuracy of performance and aging models through better understanding of the relationship between degree of lithiation and state of charge, diffusion kinetics and concentration in liquid and solid phase in the cell in operando. • No changes in objectives or approach.
Progress Report	In this quarter we fabricated a sealed electrochemical cell by employing a fast charging/discharging electrode material: lithium titanate (Li4Ti5O12, LTO), and conducted neutron depth profiling experiments. The purpose is to validate that in-situ neutron depth profiling can be used for fast charging/discharging LIB studies. The structure of the assembled cell can be found in the previous quarter report. Generally, LTO electrode replaced Sn electrode, which is regarded as one of the fast charging/discharging materials currently under studied by several institutes. The thickness of the LTO electrode is approximately 40 µm, based on SRIM simulation, only the charged particles generated from 5 µm deep into the surface can contribute to the signal. The electrolyte sandwich between the LTO and the Li metal is composed of a 25 µm Celgard (80 % porosity) immersed in a conventional carbonate electrolyte (1.0 M LiPF6 in 1:1 w/w EC: DMC), which is the channel to transport Li+ ions between the LTO electrode and the Li foil. The 300 µm Li foil serves as both the counter and reference electrode. A 7.5 micrometer Kapton® film covers the top surface of the LTO electrode sealing the cell from leaking electrochemical substances, and also stops the alpha particles avoiding signal interference of the measured triton signal. The in-situ NDP experiment was conducted at the National Institute of Standards and Technology's (NIST) Center for Neutron Research (NCNR), while all experimental design optimization was conducted at OSU's Research Reactor facility. The setup can be found in the previous report. The battery sample receives a cold neutron beam with a flux of 10^9 /cm^2-s during a controlled charging/discharging rate of C/6. NDP spectra collected during charge/discharge cycles were recorded every 5 min. The real-time evolution of the Li distribution at about 60 min intervals are shown in Fig. 1. The resolution is low thus the curves are smoothed by using 100 data average. However, the resolution can be improved by integrating the signal from multiple 5 min period NDP spectra or channels. From these results we conclude that during the charging process, 1) changes in the Li^+ ion concentrationwas observed in the bulk of the LTO sample 2) the Li^+ concentration increases uniformly and steadily within the observed region over 3 hours of lithiation. During the discharging process, 1) there is no significant change in the lithium concentration during the 1st hour of delithiation; 2) the Li^+ concentration does not decrease in uniform increments during discharging at constant C-rate but most of them were removed during the 2nd hour delithiation; 3) the Li^+ concentration deceases uniformly across the bulk during discharging. This research provides a second verification of the experimental setup developed in this project, and demonstrates that in-situ NDP can be effectively used for fast charging/discharging electrode materials studies for Lithium ion battery applications.

US-China Collaboration Activities	• None so far
Issues of Concern	• None
Notable Recent Achievements	• Danny X. Liu, Jinghui Wang, Pan Ke, Jie Qiu, Marcello Canova, Lei. R. Cao and Anne C. Co, "In Situ Quantification and Visualization of Lithium Transport with Neutrons," accepted by Angewandte Chemie International Edition

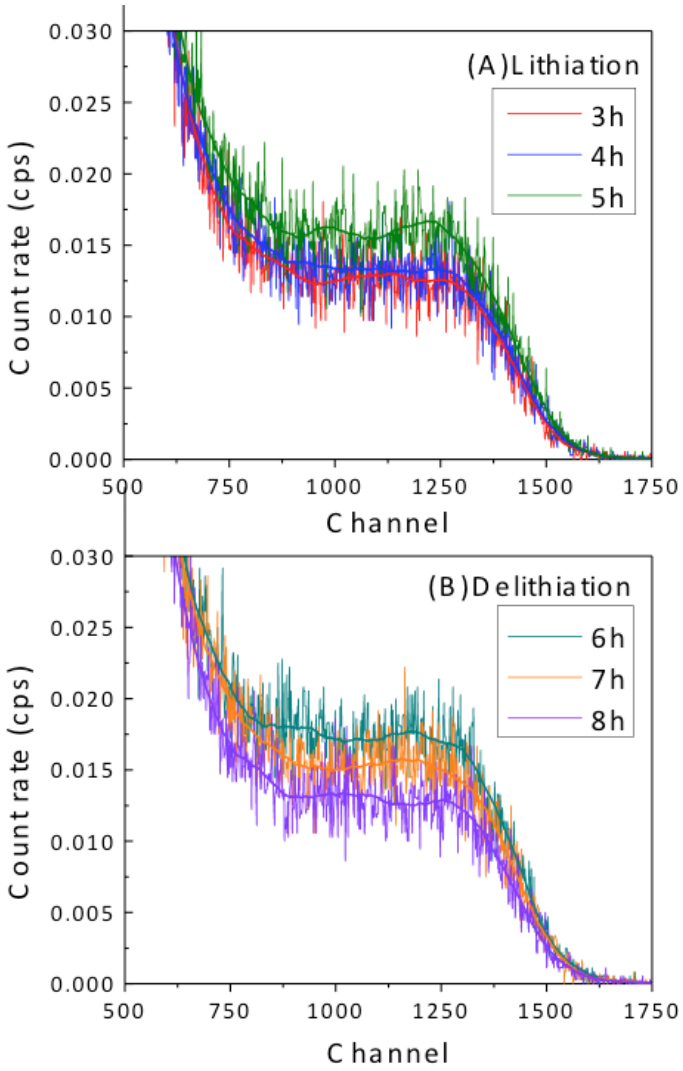


Fig. 1. In-situ NDP spectra showing Li transport during (A) charging and (B) discharging (constant rate of C/6) of the lithium titanate (Li4Ti5O12, LTO) electrodes prepared and supplied by Idaho National Lab. The plots are generated by the average the data collected over 1 hour.

Thrust	TA 1: Advanced Batteries and Energy Conversion
Title	**Project 1.3: Li-ion Battery Aging and Internal Degradation Mechanisms (US Cooperative(US))**
Personnel	PIs: Kevin Leung (Sandia), Don Siegel (UM) Postdoc Research Fellow: Nitin Kumar (UM)
Objective	• To predict atomic scale cathode degradation mechanisms for spinel $LiMn_2O_4$ oxides, a promising cathode material for lithium-ion batteries, using first principles computational methods. • A second objective is to apply similar methods to study the stability of electrolytes on Li-air cathode surfaces. This work is synergistic with Dr. Siegel's CERC high-energy density battery project.
Progress Report	The high theoretical specific energy of the Li–O_2 battery[1] makes it a promising candidate for energy storage in electric vehicles (EV). However, one of the main issues hindering the progress of Li-O_2 batteries is decomposition of the organic electrolyte[2]. The electrolyte degradation can result in high charging overpotentials, capacity fade and limited cycle life. Therefore a clear understanding of these reactions is a crucial first step in developing practical Li-O_2 batteries. We are using Van der Waals-augmented density functional theory calculations to study the initial decomposition reactions of the commonly used electrolyte solvent DME on peroxide-like and superoxide-like surfaces[3] of Li_2O_2, a primary discharge product in Li-O_2 batteries[1]. The DME molecule adsorbs more exothermally on peroxide-like than on superoxide-like surfaces. As shown in a previous cluster calculation[4], the degradation reaction proceeds exothermally via hydrogen abstraction (H-abstraction) wherein a hydrogen detaches from either primary or secondary position of DME and bonds to surface O_2 dimers. The H-abstraction results in dissociation of O_2 dimers, forming a surface hydroxyl (-OH) and a reactive oxygen that nucleophilicly attacks the H-abstracted carbon of DME. The H-abstraction reaction is significantly more exothermic on peroxide-like than on superoxide-like surface. However, the activation energy calculations show that DME decomposes more readily on superoxide-like than on peroxide-like surface. Also, the H-abstraction reaction is found to occur more easily from the secondary position of DME for both surfaces. The charge analysis on these H-abstraction reactions show a total of one electron transferred from DME molecule to the Li_2O_2 slab for both surface. On superoxide-like surface, a charge transfer from bulk peroxide moieties to surface superoxide oxygen dimers occur during the H-abstraction reaction. We have also tested the effect of solvation via continuum and explicit modelling on the reaction pathways and found it to have small influence on the reaction kinetics. 1. McCloskey, B. D. *et al.* Combining Accurate O2 and Li2O2 Assays to Separate Discharge and Charge Stability Limitations in Nonaqueous Li–O2 Batteries. *J. Phys. Chem. Lett.* **4,** 2989–2993 (2013). 2. Garcia-Araez, N. & Novák, P. Critical aspects in the development of lithium–air batteries. *J. Solid State Electrochem.* **17,** 1793–1807 (2013). 3. Radin, M. D., Rodriguez, J. F., Tian, F. & Siegel, D. J. Lithium Peroxide Surfaces Are Metallic, While Lithium Oxide Surfaces Are Not. *J. Am. Chem. Soc.* **134,** 1093–1103 (2012). 4. Assary, R. S., Lau, K. C., Amine, K., Sun, Y.-K. & Curtiss, L. A. Interactions of Dimethoxy Ethane with Li2O2 Clusters and Likely Decomposition Mechanisms for Li–O2 Batteries. *J. Phys. Chem. C* **117,** 8041–8049 (2013).

Industry Collaboration	• None
US-China Collaboration Activities	• Our computational study of degradation at LMO cathodes is synergistic with experimental studies of degradation in this same class of cathodes being performed by Prof. Qiu's group at THU and Amine's group at ANL.
Issues of Concern	• None
Notable Recent Achievements	• Poster related to this work was presented at: (1) Surface Analysis Meeting at Albuquerque, (2) Beyond Lithium Ion VII at Argonne National Laboratory, (3) BASF/University of Michigan poster session at Ann Arbor. • Manuscript in preparation for "DME decomposition on Li_2O_2 surfaces: Role of peroxide and superoxide terminations".

Thrust	TA 1: Advanced Batteries and Energy Conversion
Title	**Project 1.4: Manufacturing of Pouch Cells for Battery Degradation Studies (Joint)**
Personnel	PIs: Claus Daniel (ORNL), Jianlin Li (ORNL), David Wood III (ORNL), Shrikant C Nagpure (ORNL)
Objective	• Demonstrate manufacturing of large format pouch cells (66x99x12 mm, 100 mAh-7 Ah) • Manufacture and distribute demonstration size pouch cells to various CERC partners conducting degradation studies • Manufacture special cells with customized designs that can assist in characterization studies
Progress Report	• <u>Demonstration Size Pouch Cell:</u> – 10 1-1.3 Ah pouch cells were successfully assembled with NMC532 as cathode, A12 as anode and 1.2 $LiPF_6$ in 3:7 (by weight) EC:DMC electrolyte (A demo is shown in **Fig. 1**). – The cells demonstrated excellent and consistent performance when tested at various C-rates. The data from the average of 4 cells are shown in **Fig. 2** – All the cell processing parameter capabilities are listed in the **Appendix B**. – The established goals for this objective have been achieved successfully. • <u>Manufacturing and Distribution of Cells:</u> – The thrust area members were given updated slides that highlighted all the cell processing parameters capabilities on February 14th, 2014. The members were requested to provide feedback about the materials, capacity and cycling parameters to generate cells for degradation studies. – Separate Brainstorming session was held with OSU. Since OSU has finished aging other cells (A123 cells previously acquired) they are going to continue characterization studies on these cells with $LiFePO_4$ cathode. – Individual meetings were held with Zhili Feng (PI for Project # 1.1.4) and possibility of making different cells to support his project was discussed. A teleconference was also held with Honda to receive their feedback on this activity. We were able to draft an initial plan to manufacture cells that will support Project 1.1.4. This plan was presented to all the thrust area members during the monthly teleconference on June 25th. Ted Miller from Ford provided some valuable feedbacks for our activity. Based on the feedback from all the members the plan was further developed to include defect study. The final plan has been detailed in **Appendix C**. This final plan will be presented during the

	monthly teleconference on July 16th. The cell manufacturing according to this plan will begin in the coming quarter. The cells will be manufactured *'just in time'* when the beam time is available for Project 1.1.4 as we want to minimize the effects of shelf life on the cell performance. • <u>Custom Cells:</u> – Project # 1.1.4 (PI: Zhili Feng) needs special cells to study the background signal from various components of the cell. We will make following custom cells in the coming quarter to support Project # 1.1.4 activities: ▪ Cell # 1: Empty pouch with separator ▪ Cell # 2: Cell with *dry anodes* ▪ Cell # 3: Cell with *dry cathodes* ▪ Cell # 4: Cell with anodes, cathodes, separator and *electrolyte*
Industry Collaboration	• We have worked closely with Honda and Ford. During the quarter we had several discussions with them and their input was sought in designing the cell and preparing our plan.
US-China Collaboration Activities	• Currently our activities support US researchers conducting degradation studies. • We will meet with researchers from China during the upcoming annual meeting and discuss any possibilities of collaboration.
Issues of Concern	• Limited number of cycling channels to cycle the cells to different level of aging can be a bottleneck in supplying cells for the degradation studies along the life of the cell.
Notable Recent Achievements	• Able to reproducibly manufacture large format pouch cells with customized design to meet specific requirements of the experimental technique

<u>Appendix A</u>

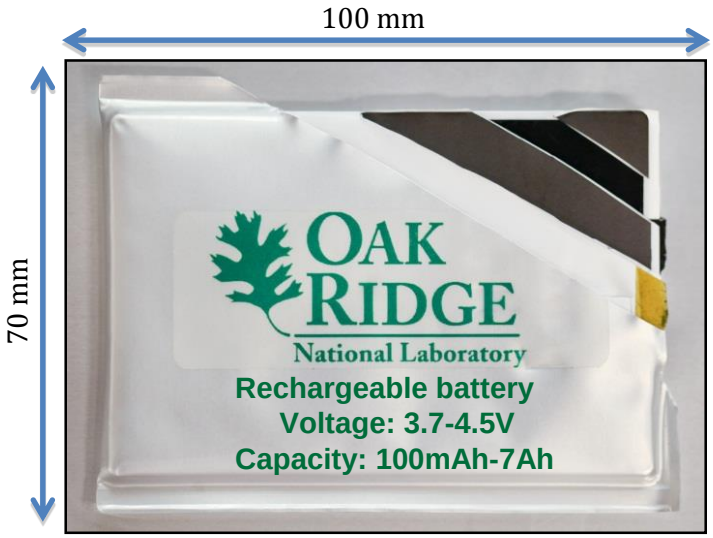


Figure 1: A demonstration of pouch cell assembled at the Battery Manufacturing Facility at Oak Ridge National Laboratory

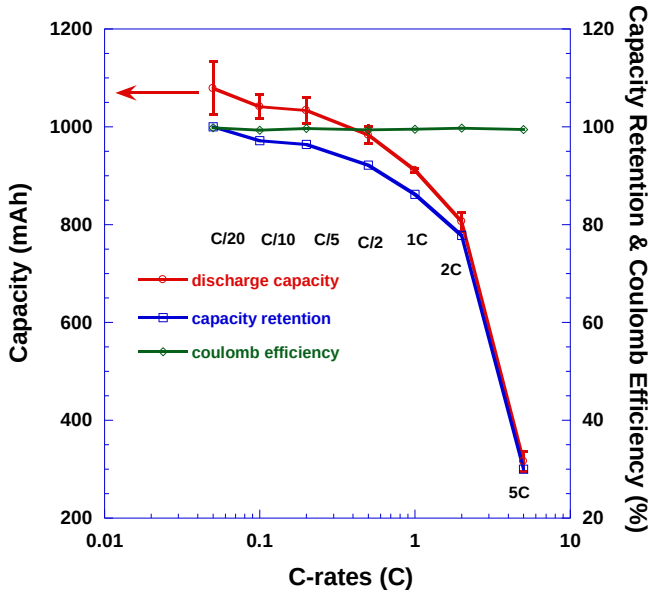


Figure 2: Rate performance, capacity retention and columbic efficiency (average of 4 1-Ah pouch cells)

Appendix B

- Standard Electrode Dimensions:
  - Cathode: 8.44 cm×5.60 cm
  - Anode: 8.64 cm×5.80 cm
  - 50-80 mAh per electrode with single side coating
- Current collector:
  - Cathode: Aluminum (15 µm)
  - Anode: Copper (10 µm)
- Capacity Range: 50 mAh to 7 Ah (typical 1.0 Ah)
- Solid loading:
  - Cathode (NMC532): 7.0-16.0 mg/cm^2 (typical 12.0 mg/cm^2)
  - Anode: 4.0-9.4 mg/cm^2 (typical 7.0 mg/cm^2)
  - Electrode Balance: N/P=1.0-1.2
- Uncalendered Electrode:
  - Cathode (NMC532 Thickness): 40-100µm
  - Anode Thickness: 40-90 µm
  - Uncalendered Porosity: ~50%

Appendix C

Cell Specifications:

- Anode:
  A12 Graphite (Conoco Philips)/carbon black/PVDF (in NMP) binder = 92/2/6 weight%
  Solid loading in dispersion: 40 weight%
- Cathode:
  NMC532 (Toda America)/carbon black/PVDF (in NMP) binder = 90/5/5 weight%
  Solid loading in dispersion: 45 weight%
- Electrolyte:
  1.2 M $LiPF_6$ in 3:7 EC:DMC (by weight)
- Capacity: 1 Ah

Cell Manufacturing:

1. Inhomogeneities and Initial Capacity Fade:
   a. In-situ testing of 3 cells with formation cycle protocol proposed by ANL

    b. In-situ testing of 3 cells with formation cycle protocol with 20% higher current density
2. Long Term Performance:
    a. In-situ analysis of set of 3 cells formed with ANL protocol and aged with USABC DST_{620} cycling protocol for 500 cycles.
    b. In-situ analysis of set of 3 cells formed with 20% higher current density protocol and aged with USABC DST_{620} cycling protocol for 500 cycles.
    c. In-situ analysis of set of 3 cells formed with ANL protocol and aged with USABC DST_{620} cycling protocol for 1000 cycles.
    d. In-situ analysis of set of 3 cells formed with 20% higher current density protocol and aged with USABC DST_{620} cycling protocol for 1000 cycles.
3. Defective Electrode:
    a. In-situ analysis of 3 cells assembled with electrodes having known defects to study the evolution of structure in defective electrodes during aging.
    b. In-situ analysis of 3 cells assembled with electrodes having gradient in solid loading along the length and study effect of variability in cell manufacturing and solid electrolyte formation (SEI)
4. Different Processing Methods:
    a. In-situ testing of 3 cells with electrodes manufactured using aqueous processing method and formed with protocol proposed by ANL
    b. In-situ testing of 3 cells with electrodes manufactured using aqueous processing method and formed with 20% higher current density

Thrust	TA 1: Advanced Batteries and Energy Conversion
Title	**Project 2.1: Advanced Battery Chemistries (Joint)**
Personnel	PIs: Don Siegel (UM), Feng Wu (BIT), Borong Wu (BIT), Xiang-Ming He (THU) Graduate students: Sheng Yang (UM) Visiting scholar: Junichi Naruse (Denso)
Objective	• Identify of mechanisms that limit the performance of metal-air batteries, including: high charging potentials, poor reversibility, and limited capacity/capacity fade. • Perform first principles calculations to reveal the mechanisms and efficiency of charge transport in metal air cathodes.
Progress Report	• We are continuing our research into the mechanisms for charge transport in the primary discharge phases in Na-O2 batteries: Na_2O_2 and NaO_2. Our previous calculations revealed that hole polarons and negative sodium vacancies are the dominant charge-carrying species in both Na_2O_2 and NaO_2. Hole polaron are formed when a hole (missing electron) is trapped on O_2 dimers, occupying the π^* state. The concentration of these carriers is slightly higher concentration in NaO_2 than in Na_2O_2. • Electronic conductivity in Na_xO_y can arise from the hopping of small hole polarons. We used the nudged elastic band (NEB) method to evaluate the energy barrier associated with polaron hopping between O_2 dimers. These barriers are an essential ingredient in estimating the polaron's mobility. We found that the hopping barriers in Na_2O_2 and NaO_2 are comparable. Combining the concentration and mobility data, we estimate that the electronic conductivity in NaO_2 is three orders higher than Na_2O_2, but still low overall, consistent with insulating behavior. • The comparable conductivities for Na_2O_2 and NaO_2 suggest that enhanced bulk charge transport is not responsible for lower charging overpotentials in Na-air cells that discharge to NaO_2.
Industry Collaboration	• Continued to collaborate with CERC industry partner DENSO by hosting visiting scholar Junichi Naruse
US-China Collaboration Activities	
Issues of Concern	
Notable Recent Achievements	Delivered two invited presentations that acknowledge CERC funding: 3. 1st International Symposium on Sustainable Secondary Battery Manufacturing and Recycling, June 29-July 4, 2014, Cancun, Mexico 4. U.S. Nat. Congress on Theoretical and Applied Mechanics, June 15-20, 2014, East Lansing, MI Two posters presented at Beyond Lithium Ion 7 Conference that acknowledge CERC funding: 2. Nitin Kumar, Maxwell D. Radin, D. J. Siegel, "DME Decomposition on Li2O2 Surfaces: Peroxide vs. Superoxide Terminations," Beyond Lithium Ion VII, Argonne, Illinois, June 3-5 2014 3. Sheng Yang and D. J. Siegel "Charge transport in Na-O2 batteries," Beyond Lithium Ion VII, Argonne, Illinois, June 3-5 2014

Thrust	TA 1: Advanced Batteries and Energy Conversion
Title	**Project 2: Fundamental Understanding of Li-Air Reaction Mechanisms**
Personnel	PIs: Yang Shao-Horn and Gerbrand Ceder (MIT) Graduate students: David Kwabi (50%) and ShinYoung Kang (50%) (MIT)
Objective	Metal−O_2 batteries are being heavily investigated for their higher theoretical energy densities than Li-ion batteries, but widescale adoption is hampered due to device-level limitations such as low round-trip efficiency and poor cycle life. Our aim is to understand the fundamental reaction mechanisms in Li−O_2 and Na-O_2 cells, and possible effects on parasitic reactions that can be detrimental to battery performance. • Investigate species responsible for decomposition of discharge products in Li-O_2 batteries with dimethylsulfoxide (DMSO)-based electrolytes and characterize decomposition products using x-ray diffraction (XRD) and Raman and Fourier-transform infrared (FTIR) spectroscopies. • Study the thermodynamic stability and phase diagrams of various bulk sodium oxides (e.g. Na_2O, Na_2O_2, NaO_2 and NaO_3) using first-principles calculations.
Progress Report	• We found that the expected Li_2O_2 discharge product is present immediately after discharge in a DMSO-based electrolyte, but decomposes upon prolonged contact with the electrolyte into LiOH, and that this process is accompanied by DMSO decomposition. • Using XRD, mass spectrometry and Raman and FTIR spectroscopies, the chemical reactivity of commercial KO_2 and Li_2O_2 powders with DMSO was investigated, and showed that the instability of Li_2O_2 in contact with DMSO is greatly enhanced by the presence of superoxide anions in KO_2, highlighting the unique role of superoxide species in acceleration parasitic reactions in Li-O_2 cells. • Na-O phase diagram studies show that although Na_2O_2 is a stable phase in bulk at the standard state (300 K, P_{O2} = 1 atm), nano-scale low surface energies stabilize NaO_2 nano-particles up to 6 nm at the standard state.
Industry Collaboration	• Collaborating with scientists at Liox Power (Pasadena, CA) investigating the effects of Li^+ and O_2^- ion solvation on redox reactions in Li-O_2 cells.
US-China Collaboration Activities	N/A
Issues of Concern	N/A
Notable Recent Achievements	Kwabi, D.G., Batcho, T.P., Amanchukwu, C.V., Ortiz-Vitoriano, N., Hammond, P., Thompson, C.V., Shao-Horn, Y. (2014). "Chemical Stability of dimethyl sulfoxide in lithium-air batteries" *Submitted for publication*

Thrust Area 2: Clean Combustion and Energy Conversion

Thrust	Thrust 2: Advanced Biofuels, Clean Combustion and Auxiliary Power Unit (APU)
Title	**Project 1.1: Biofuel Chemistry & Physics (Cooperative)**
Personnel	PIs: Angela Violi (UM), Craig A. Taatjes (Sandia), Blake A. Simmons (JBEI, Sandia) Research Scientists: Brandon Rotavera (Sandia), Mohamad Akbar Ali (UM)
Objective	• Characterize fundamental ignition-related chemistry of large, structurally-complex biofuels produced using microbial synthesis using combined experimental and computational approach • New target fuels: farnesane, *ortho*-xylene, *meta*- xylene, *para*- xylene • Determination of the effect of temperature on competing chain-propagation and -termination channels to contribute to fundamental combustion modeling efforts

Progress Report	• Seven molecules studied to-date: (1) 2,5-dimethylhexane; (2-4) o-/m-/p-cymene; (5-7) o-/m-/p-xylene
	• Expanded prior CERC-funded investigation into 3 key features related to a low-temperature ignition phenomena characteristic of some substituted aromatics (the *ortho*- effect) which are relevant to diesel and gasoline applications (see list below). These results are the first of their kind, and can have significant impact on the fundamental understanding of the initial steps of substituted aromatic oxidation.
	  ○ Temperature-dependence of the *ortho*- effect in cymenes and in xylenes
	  ○ Studied primary low-temperature fuel consumption pathways using branching fraction measurements performed at the Advanced Light Source of Lawrence Berkeley National Laboratory
	• **Journal paper** accepted which included results from cymene experiments and modeling (journal: *Proceedings of the Combustion Institute*, ISSN: 1540-7489)
	• Completed: calculations of all R + O_2 stationary point energies (*ortho*-cymene)
	• Completed: Laser-absorption measurements of OH and HO_2 time histories of previous CERC fuel (2,5-dimethylhexane)
	• **Manuscript** ready for submission (part 1 of 2 papers on 2,5-dimethylhexane); main results: (1) photoionization mass spectrometry measurements of initial oxidation steps, (2) *ab inito* calculations of rate coefficients.
	• **Manuscript** being finalized (part 2 of 2 papers on 2,5-dimethylhexane); main results: (1) improved modeling of 2,5-dimethylhexane oxidation using Master Equation computation of rate coefficients, (2) successful modeling of OH/HO_2

Industry Collaboration	• None; collaboration involved national laboratory (Sandia) and academia (U. Mich)
US-China Collaboration Activities	• Productive, monthly phone meetings with all U.S./China CERC collaborators ○ Discussions focused on common biofuel to target for potential CERC 2 projects, including (1) farnesane and (2) *iso*-pentanol • Post-doctoral fellows trained (Rotavera, Sandia; Ali, U. Michigan)
Issues of Concern	None
Notable Recent Achievements	Describe any product produced or tech transfer activity such as: • Journal publication on cymene oxidation to be presented at the biannual 35th International Symposium on Combustion (held in August 2014) • Completed preliminary testing of high-pressure experimental apparatus for performing fundamental ignition-relevant fundamental chemistry measurements of low-vapor-pressure biofuels (e.g. cymenes, bisabolane).

Thrust	Thrust 2: Advanced Biofuels, Clean Combustion and Auxiliary Power Unit (APU)
Title	**Project 1.2: Chemical and Physical Models for Novel Biofuels**
Personnel	PI: Prof. Angela Violi, Associate Professor, Department of Mechanical Engineering, University of Michigan Graduate Students: Shao Teng Chong, M.S. Student (UM ME dept) Tyler Dillstrom, Ph.D. Student (UM ME dept) Visiting Scholar: Tanjin He, Tsinghua University, China
Objective	The objective of this project is to develop chemical kinetic mechanisms for novel bio-derived fuel molecules such as bisabolane and farnesane by characterizing the chemistry of the ignition and chain propogation/branching fractions.
Progress Report	An important component of the combustion research process is computational modeling of the in-engine behavior of fuels. As such, there is interest in developing accurate and reliable reactions models for these novel bio-derived hydrocarbon fuels. However, due to the structural complexity of the bio-derived fuels of interest, namely bisabolane and farnesane, we use a component-centered approach to explore the chemistry of fragments of said fuels and proceed to piece together the chemical kinetics of the various fragments in order to create a kinetic mechanism for bisabolane and farnesane. Previously, we explored both the low and high temperature oxidation of 2,5-dimethylheptane (a bisabolane fragment). This enabled us the create a sub-mechanism that described the pyrolysis and oxidation of 2,5-dimethylheptane. We then incorporated that sub-mechanism into a generic hydrocarbon mechanism. This allowed us to simulate combustion phenomena from experimental apparatuses like shock tubes and rapid compression machines. This work led to a manuscript that is currently in preparation and is expected to be submitted by the fall. This quarter was focused on developing a refined mechanism that we could use to model lab-scale experiments. These simulations, along with the quantum chemistry calculations that yielded the kinetic rates, were the basis of the manuscript currently in preparation. The manuscript relates our work to the community in a manner consistent with both papers that concern kinetic rates developed via quantum chemistry methods as well as combustion papers that focus on developing kinetic models. The relative uniqueness of our paper is that it combines both disciplines in order to describe the process of developing a kinetic mechanism for a novel fuel from the bottom up. Future work will focus on developing the chemistry of 2,6-dimethylheptane, a component of farnesane. We intend to develop a fully refined kinetic mechanism for farnesane in a similar manner to the work with 2,5-dimethylhexane.
Issues of Concern	N/A
US-China Collaboration Activities	Monthly Conference calls Since February a visiting scholar from Tsinghua University has been working with us. This has increased the level of collaboration with China. Additionally there are plans to coordinate with Prof. Xin He at Tsinghua University on experiments.

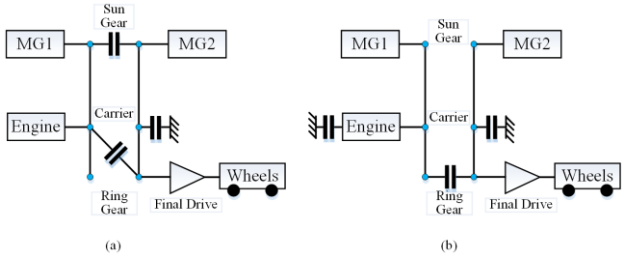
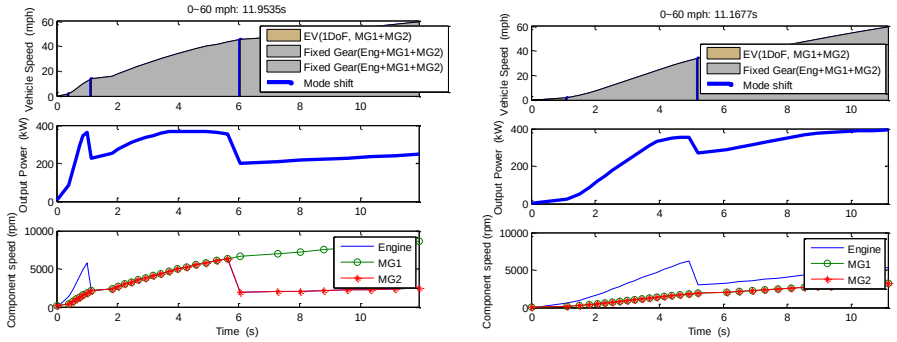
Industry Collaborators	Collaborations with Sandia National Lab and Tsinghua University in China.
Notable Recent Achievements	**Conferences and Meetings:** (Acknowledgements to CERC-CVC) 1. Mohamad Akbar Ali and Angela Violi, Unimolecular decomposition reaction of biofuel, **US-China CERC, Michigan, Ann Arbor, USA, 27-28 August, 2012.** 2. Mohamad Akbar Ali and Angela Violi, Theoretical study of thermal decomposition of biodiesels fuels, **22nd International Symposium on Gas Kinetics, Boulder, Colorado, USA, 18-22 June 2012.** 3. Mohamad Akbar Ali, V. Tyler Dillstrom, Jason Y. W. Lai and Angela Violi, Ab Initio Investigation of the Thermal Decomposition of n-Butylcyclohexane, **34th International Symposium on Combustion Warsaw, Poland, 29th July- 3rd August 2012.** 4. Brandon Rotavera, Mohamad A. Ali, Oliver Welz, Leonid Sheps, Adam M. Scheer, John D. Savee, David L. Osborn, Taek Soon Lee, Angela Violi, Blake A. Simmons, and Craig A. Taatjes, Component-centered approach towards oxidations studies of complex biofuels. **8th International Conference on Chemical Kinetics, Spain 8th -12th July, 2013.** **Research Article** 1. Reaction Pathways for the Thermal Decomposition of Methyl Butanoate. Mohamad Akbar Ali and Angela Violi, *Journal of Organic Chemistry* 78(12), pp. 5898-5908 (2013) 2. Ab Initio Investigation of the Thermal Decomposition of n-Butylcyclohexane. Mohamad Akbar Ali, V. Tyler Dillstrom, Jason Y. W. Lai and Angela Violi *The Journal of Physical Chemistry A* 118 pp. 1067-1076 (2014)

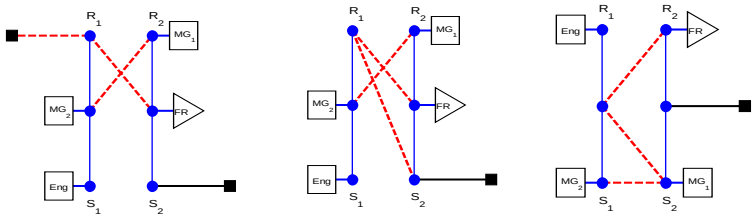
Thrust	TA 2: Advanced Biofules and Clean Combustion
Title	**Project 2: Integrated Powertrain and Aftertreatment System Control for Clean Vehicles (Joint)**
Personnel	PI: Junmin Wang (OSU), Jim Parks (ORNL), Fuyuan Yang (THU), Graduate student: Junfeng Zhao (OSU)
Objective	The objective of this project is to develop synergistically-integrated, systematic, optimal, and generalizable control methodologies for clean vehicle Diesel powertrain systems. Such control systems will optimally coordinate fuel property estimation, advanced combustion modes, exhaust aftertreatment systems, and hybrid powertrains to enable maximization of the energy efficiency and emission reduction potentials for clean vehicles.
Progress Report	• Experimentally studied the effects of Diesel and biodiesel fuel during DPF active regenerations. • Researched on methods for active thermal management of aftertreatment systems. • Developed control methods for hybrid electric vehicles considering the aftertreatment systems and emissions requirements.
Industry Collaboration	• We have involved CERC-CVC industry partners in the Annual Conference in August 2013, and the inputs from industry are being taking into consideration in this research project.
US-China Collaboration Activities	-Research discussions and exchange visits are being planned. -Prof. Junmin Wang will visit Tsinghua University again to discuss on the collaborations in July 2014 -We also discussed research collaborations with China partners at the CERC-CVC Annual Conference in August 2013, and through conference calls.
Issues of Concern	No major issues
Notable Recent Achievements	1. Pingen Chen, Umar Ibrahim, and Junmin Wang, "Experimental Investigation of Diesel and Biodiesel Post Injections during Active Diesel Particulate Filter Regenerations," *Fuel*, Vol. 130, pp. 286 - 295, 2014. 2. Junfeng Zhao and Junmin Wang, “Model Predictive Control of Integrated Hybrid Electric Powertrains Coupled with Aftertreatment Systems” *Proceedings of the 2014 ASME Dynamic Systems and Control Conference*, 2014 (accepted). •

Thrust	TA 2: Advanced Biofules and Clean Combustion
Title	**Project 4: Energy Conversion-Efficient TE Materials for Vehicle Waste Heat Recovery (joint)**
Personnel	PIs: Ctirad Uher (UM), Rachel Goldman (UM), Kevin Pipe (UM), Joseph Heremans (OSU), Douglas Medlin (Sandia), Hsin Wang (ORNL), Xinfeng Tang (WHUT), Han Li (WHUT) Graduate students: Si Hui (UM), Jenna Walrath (UM), Michele Nielsen (OSU), Postdoctoral researcher: Dr. Yen-Hsiang Lin (UM)
Objective	• Develop new, efficient TE materials for waste heat recovery in cars and trucks. • Develop tools for characterization of homogeneity of TE materials. • No changes in research objectives.
Progress Report	1. Completed transport measurements on Sn-doped, p-type $Yb_xFe_4Sb_{12}$ skutterudites. Oral report presented at the ICT2014 in Nashville, July 9, 2014. 2. Explored p-type doping by aluminum on the sites of antimony in $CoSb_3$ skutterudites. Aluminum doped samples show greatly improved Seebeck coefficients over a wide range of carrier concentrations as attested to by the Pisarenko plot shown on the slide. Oral report presented at the ICT2014 in Nashville, July 9, 2014. 3. Novel synthesis route based on self-propagating high temperature synthesis (SHS) is being applied to preparation of thermoelectric materials jointly at WHUT and UM. An invited talk given at the ICT2014 in Nashville, July 8, 2014. 4. Performed 3D band structure simulations and Seebeck coefficient calculations of Stranski-Krastanow InAs/GaAs quantum dots. The data reveal that maxima of the Seebeck coefficient at the edges of the quantum dots are due to band bending-induced interfacial charge accumulation. 5. Converted measured Seebeck coefficient to a local carrier concentration of InAs/GaAs quantum dot and wetting layer. The carrier concentration is lower inside the quantum dot than in the wetting layer.
Industry Collaboration	None, but discussions with potential industrial partners in progress.
US-China Collaboration Activities	Prof. Uher visited the Wuhan University of Technology during May 23-June 3, 2014.
Issues of Concern	None
Notable Recent Achievements	• W. Liu, H. Chi, H. Sun, Q. Zhang, K. Yin, X. F. Tang, Q. Zhang, and C. Uher, "Advanced Thermoelectrics Governed by Single Parabolic Band: $Mg_2Si_{0.3}Sn_{0.7}$, a Canonical Example", *Phys. Chem. Chem. Phys*. **16**, 6893-6897 (2014). • X. F. Tang, X. Su, F. Fu, Y. Yan, and C. Uher, "Combustion Synthesis Applied to Compound Thermoelectric Semiconductors: a New Criterion for Applicability of Combustion Processing", an invited talk at the International Conference on Thermoelectrics, Nashville, July 8, 2014. • S. Hui, J. R. Salvador, K. P. Pipe, and C. Uher, "Effect of Sn Dopants on the Thermoelectric Properties of p-type Yb-filled Skutterudites", an oral presentation at the International Conference on Thermoelectrics, Nashville, July 9, 2014. • M. J. Adams, M. D. Nielsen, and J. P. Heremans, "Improving Electronic Properties of Al-doped CoSb3", an oral presentation at the International Conference on Thermoelectrics, Nashville, July 9, 2014.

Thrust Area 3: Vehicle Electrification

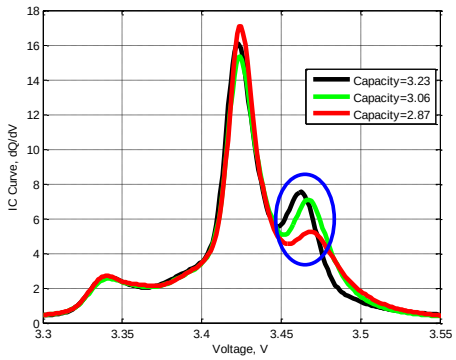
Thrust	TA 3: Vehicle electrification
Title	**Project 1: Efficient and high-power density electric powertrain (Joint)**
Personnel	PIs: Heath Hofmann (UM) Graduate students: Jason Pries (UM)
Objective	The objective of this project is to develop computationally-efficient finite-element-based steady-state solvers for electric machines. Our approach has changed slightly, in that we have traded the development of 3D techniques which accurately capture core losses for the development of algorithms that are readily parallelizable.
Progress Report	A revision of our project's MATLAB toolbox is underway in order to allow more flexibility in the investigation of different winding structures, source types, and external circuits. The update is expected to be completed by the end of July. This result is in sync with the time-line for Task 1.1.5. Jason Pries is midway through a six-month stay at Oak Ridge National Lab's National Transportation Research Center as a visiting scholar, where he has been interacting with Tim Burress of the Power Electronics & Electric Machinery Research Center. ORNL is interested in using our codes for electric machine design and optimization. Our next step will be to implement a parallel version of our previously developed harmonic balance/domain decomposition algorithm for synchronous machines. Subsequently, our focus will turn towards implementing versions of our time-domain and frequency domain solvers for asynchronous machines. These solvers will exploit the poly-phase time-periodic condition (time-domain) and the 2D-DFT method (frequency-domain). The previously mentioned toolbox update will allow straightforward modeling of the asynchronous machine rotor topology. The toolbox is structured in a general manner with respect to the stator source type; so that all work on task 1.1.6 is applicable to task 1.1.4.
Industry Collaboration	In a separate project, funded by DENSO, a CERC member, we are using this code to design an electric machine for a traction drive in electric vehicles. A prototype of the machine design is currently under construction. We are also using this code to validate the performance of an electric machine we have developed under a project supported by the Bosch Energy Research Network.
US-China Collaboration Activities	Ziyou Song, a student from Tsinghua University in Beijing, is spending 2014 with our research group as a visiting scholar. This collaboration has resulted in multiple journal paper submissions.
Issues of Concern	None.
Notable Recent Achievements	Our paper entitled *"Steady-State Algorithms for Nonlinear Time-Periodic Magnetic Diffusion Problems using Diagonally-Implicit Runge-Kutta Methods"* has been accepted for publication, pending revisions, by IEEE Transactions on Magnetics.

Thrust	TA3: Vehicle Electrification
Title	**Project 3.1 System integration technologies for improved efficiency, safety, reliability and NVH performance (Joint)** Task 1- A systematic design procedure for double planetary hybrid vehicles
Personnel	PIs: Prof. Huei Peng (UM), Prof.Jing Sun (UM), Prof. Giorgio Rizzoni (OSU), Prof. Jianqiu Li (THU) Dr. Liangfei Xu (THU), Prof. Chengliang Yin (SJTU), Prof. Li Chen (SJTU) Graduate Students: Xiaowu Zhang (UM), Andrea Cordoba (OSU), Jiyu Zhang (OSU)
Objective	The objective of this project is to develop vehicle models as well as design and control tools for the system integration, diagnosis of electric power-trains, and NVH performance analysis. The ultimate goal is to enable rapid power-train designs and integration that are reliable and achieve optimal efficiency for clean vehicles.
Progress Report	• In the previous quarter, we extended the systematic design procedure for the hybrid vehicle with double planetary gear to designs with multiple planetary gears and clutches. All possible configurations and clutch locations can be calculated systematically. Rather than two PG, the methodology is more universal to cover the powertrain systems with arbitrary number of planetary gears, including Ravignaux planetary gears. We combined PEARS – a fast optimization method developed earlier in this project, together with an automatic modeling and mode identification approach to find the optimal clutch location for configuration #83 – A double PG configuration which was used by Toyota Prius 2010. Two example designs are shown below:  • Over the last quarter, we thoroughly searched the design space of double planetary gear system with all possible clutch locations. All 144 configurations with engine and final drive on separate PG are analyzed. • At the suggestion of our Ford collaborators, we considered drivability as the primary screening criterion and developed a systematic methodology to analyze the drivability of this vehicle under towing, climbing and acceleration. • For the acceleration evaluation, a novel power-based algorithm is developed which can be used to rapidly compute the optimal input of the powertrain component to achieve the best acceleration performance. Optimal mode selection is included in the decision process. The following two figures shows example optimal acceleration trajectory for two different designs. 

	• A plotting code is developed which can draw the lever diagram of any selected design automatically, helping developers to visually see the designs. The following figures present some of the feasible designs screened by the drivability constraint:  • The research on HEV mode shift feasibility and smoothness was initiated over the last quarter. The goal is to develop practical mode shift logic.
Industry Collaboration	• We are collaborating with Ford (Ming Kuang and Mark Jennings) on a "pathways to implementation" project, which aims to develop a power-split hybrid design for the F150 truck
US-China Collaboration Activities	• Monthly technical meetings have been arranged and WebEx meetings have allowed researchers to participate remotely. • Two students, Ziyou Song and Xuning Feng from Tsinghua University are visit Ann Arbor for a one-year exchange.
Issues of Concern	N/A
Notable Recent Achievements	- ACC 2013 Best Paper Award by the ASME Dynamic Systems & Control Division in Automotive and Transportation Systems - Xiaowu Zhang, Huei Peng, Jing Sun, "A Near-Optimal Power Management Strategy for Rapid Component Sizing of Power Split Hybrid Vehicles with Multiple Operating Modes", 2013 American Control Conference, Washington DC. - Journal Paper Accepted: Xiaowu Zhang, Huei Peng, Jing Sun, "A Near-Optimal Power Management Strategy for Rapid Component Sizing of Multi-mode Power Split Hybrid Vehicles", IEEE Transactions of Control System Technology - Conference Paper Accepted: Xiaowu Zhang, Huei Peng, Jing Sun, "Automated Modeling and Mode Screening for Exhaustive Search of Double-Planetary-Gear Power Split Hybrid Powertrains", 2014 Dynamic System and Control Conference, Santino, TX

Thrust	TA 3: Vehicle Electrification
Title	**Project 3: System integration technologies for improved efficiency, safety, reliability and NVH performance** Task 3.2. Intelligent Fault Diagnosis and Prognosis (Joint)
Personnel	PI: Prof. Giorgio Rizzoni (OSU) coPI: Prof. Hongmei Li (HFUT) Research Associate: Dr. Andrea Cordoba Arenas (OSU), Dr. Qadeer Ahmed (OSU) Graduate students: Jiyu Zhang (OSU) Visiting scholar: Associate Prof. Qi Chen (HFUT), Zhentong Liu (Beijing Institute of Technology, Ph.D student)
Objective	• To develop diagnostic and prognostic methods, algorithms and procedures for electrified powertrains to guarantee safe and reliable operation • To develop software tools to enable a suite of diagnostic and prognostic functions for the main subsystems and components comprising an electrified powertrain. • To experimentally demonstrate the methods and tools on an experimental vehicle, in collaboration with industrial partners
Progress Report	• We have been working on the development of structural analysis based FDI scheme for EcoCAR2 AMT. After the sensors placement analysis, we are working how to validate the FDI system on actual EcoCAR2 AMT. • We are also working on model based fault diagnosis of battery systems. We are able to develop a model based FDI scheme for battery cell and a battery pack of 2P2S configuration. Experimental evaluation of FDI scheme for battery cell system has been done. • We have also applied the FDI scheme based on structural analysis for PMSM drive system in an electric vehicle. We have analyzed the detectability and isolability of various type of faults that are common for PMSM drive system and derived sequential residual generators to achieve fault detection and isolation. We have tested the residual generators in Matlab/Simulink, the next step will be implement the FDI strategy in SIL and HIL environment and finally validate our diagnostic scheme in real vehicles.
Industry Collaboration	This project is part of a selected group viewed as likely to result in a commercializable output. We are working in partnership with Delphi on a two-year "path to commercialization" project with following objectives: • To propose a systematic structural-based FDI methodology to enable fail-safe architectures, fault-tolerant control and limp-home operation of electrified power trains. One of the novelties of the proposed approach is that we are going to tie the diagnostics development to the control development process. • To translate the proposed structural FDI into a process that implements the ISO26262 or some aspects thereof. • To demonstrate the proposed structural FDI process as part of the standard software tool chain that is used today to implement rapid control prototyping using as testbed the OSU EcoCAR2/3. • To translate the structural FDI concepts into some application(s) of interest to Delphi. Application #1: Unintended acceleration (vehicle safety application). Application #2 (optional): Subset of gasoline OBDII.
US-China Collaboration Activities	• Prof. Rizzoni visited Hefei in April 2014 to continue collaboration with China. • Two visiting scholars Dr. Qi Chen and Zhentong Liu have joined in this project. Dr. Chen is working on modeling of EcoCAR2 Automated Manual Transmission, its fault diagnosis, and fault tolerant control. Zhentong Liu is working on battery hazard analysis and fault diagnosis, in collaboration with EcoCAR2. • Ph.D student Jiyu Zhang visited HFUT in July 2014 to continue collaboration with Prof. Hongmei Li's team.

	• The project team has participated in the monthly TA3 China-USA Webex meetings. In addition, the OSU team meets on a weekly basis.
Issues of Concern	There are no issues of concern in this project so far.
Notable Recent Achievements	This project is part of a selected group viewed as likely to result in a commercializable output. We are currently working in partnership with Delphi. We have already defined the commercialization path in a proposal that is been developed during several discussions between OSU and Delphi. The proposal establishes the objectives, methods and expected outcomes for the next two years collaboration. Journal Publications: 1. Cordoba-Arenas, A., Onori, S., Giorgio, G., "An experimentally validated PHEV life-cycle model for lithium-ion battery cells containing LMO-NMC positive electrodes". *Submitted to Journal of Power Sources.* 2. Cordoba-Arenas, A., Onori, S., Giorgio, G., "A control-oriented lithium-ion battery pack model for aging propagation studies". *Submitted to Journal of Power Sources.* Conference Publications: *1.* Zhentong Liu, Qadeer Ahmed, Giorgio Rizzoni, and Hongwen He, "System Level Fault Detection and Isolation Scheme for Lithium-Ion Battery Pack". s*ubmitted at CDC 2014* 2. Zhentong Liu, Qadeer Ahmed, Giorgio Rizzoni, and Hongwen He, "Fault Detection And Isolation For Lithium-Ion Battery System Using Structural Analysis And Sequential Residual Generation". *To be presented at DSCC 2014* *3.* Qi Chen, Qadeer Ahmed and Giorgio Rizzoni, "Sensor Placement Analysis For Fault Detectability And Isolability Of An Automated Manual". *To be presented at DSCC 2014* *4.* Jiyu Zhang, Andrea Cordoba-Arenas, Giorgio Rizzoni, "Fault Diagnosis for PMSM Drive System in Electric Vehicle". *To be presented at DSCC 2014* 5. Jiyu Zhang, Giorgio Rizzoni, "Structural Analysis for FDI of PMSM Drive System in Electric Vehicles". *To be presented at ITEC Asia 2014*

Thrust	TA 3: Vehicle Electrification
Title	**Project 4.1: Adaptive battery management system on and off the grid (Joint)**
Personnel	PIs: Jing Sun (UM), Huei Peng (UM) Graduate student: Caihao Weng (UM)
Objective	• To develop intelligent monitoring (while driving), diagnosis /prognosis and conditioning (while connected with grid) strategies to improve reliability, performance, and life cycle of battery systems.
Progress Report	For the second quarter of 2014, the team continued the research effort on developing effective and robust system identification algorithms for on-line detection of battery state of health for real-time monitoring, diagnosis, and prognosis purposes. In our previous work, an incremental capacity analysis (ICA) based battery state-of-health (SOH) framework was established for estimating lithium ion battery capacity degradation. An SVR based parametrization and adaptation method has also been developed for the on-board implementation of our battery SOH monitoring framework. Given the success of our framework in single battery cell application, we are now extending our method to battery module/pack SOH monitoring. Our research activities in the second quarter of 2014 have been focused on (a) Design and experimental set up for battery module testing; (b) Application of ICA based battery SOH monitoring to battery module data; (c) Aging tests for validation/ calibration of battery pack model. For part (a) and (b), 24 battery cells with different aging conditions were collected to establish a cell inventory. The cells are selected randomly to construct parallel connected 3-cell battery modules. The 3-cell battery modules were then tested using charaterization load profiles and the charging data were obtained for ICA study. As shown in Fig. 1, the IC peaks of battery modules also show a clear decreasing trend as module capacity reduces. Therefore, same as the single cell case, the correlation between IC peak value and battery capacity degradation can be used to estimate battery module capacity loss. The correlation obtained from our battery module testing data is shown in Fig. 2.  **Figure 1 IC curves of 3-cell battery modules**

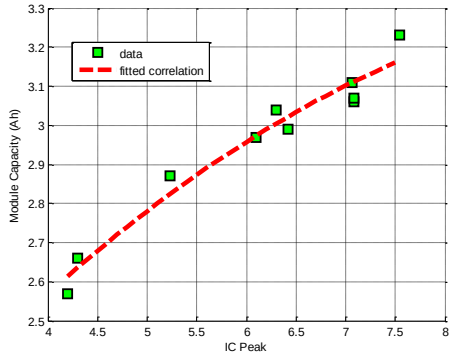


Figure 2 Correlation between IC peak value and battery capacity

For part (c), the testing set up is modified so that the current of each cell branch in the parallel connected battery module could be monitored. One 1-mOh resistor is connected in series with each cell and the branch current is collected through the measurement of resistor voltage (see Fig. 3). The resistance values are very small so that the current distribution in the battery module is not affected. The current measurement from the test data is then compared with our battery pack model for validation and calibration. The tests will continue until a battery pack model incorporating degradation mechanism could be built.

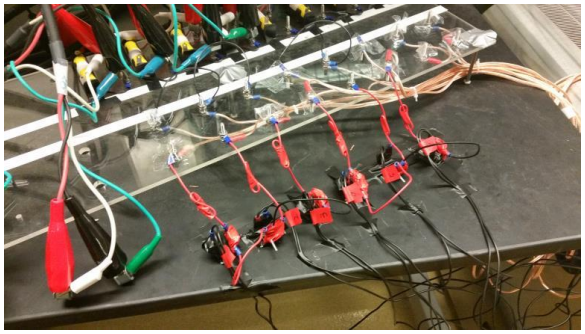


Figure 3 Experimental set up for battery module test with branch current measurement

In the next quarter, the team will continue to focus on the development of adaptive battery management system. Efforts will be directed to the study of battery degradation model. The battery pack model will be combined with cell degradation model to predict the aging mechanism of parallel connected battery cells. The results will be used to develop off-the-grid battery health management strategy.

Industry Collaboration	
US-China Collaboration Activities	• Mr. Xuning Feng, a graduate student from Tsinghua University, is visiting the University of Michigan and working with the PI.
Issues of Concern	
Notable Recent Achievements	• A paper based on the results reported here was submitted to IEEE Transactions on Vehicular Technology.

Thrust	TA 3: Vehicle Electrification
Title	**Project 4.2: Data-Based Techniques for Battery-Health Prediction (US Cooperative)**
Personnel	PIs: Dennis S. Bernstein (UM), Jeff L. Stein (UM) Research Scientists: Tulga Ersal (UM) Graduate students: Xin Zhou (UM)
Objective	• Develop and demonstrate a novel, noninvasive approach to battery diagnostics. This approach uses data obtained from only noninvasive measurements to estimate health-relevant features of a battery that are otherwise hidden. • Using numerical computation, apply the new battery diagnostic algorithm to models of Li-Ion batteries to estimate features of the battery-health subsystem. The research objective is to assess the accuracy of the algorithm under realistic modeling errors and data limitations. • Using laboratory experiments validate the ability of the algorithm with noninvasive data to make accurate assessments and predictions of battery health.
Progress Report	• Developed a new estimator, the Two Step Filter, to address the issue of high sensitivity to initialization error. Initialization errors pose an important problem because of their persistence due to the combination of the fact that the battery, being an energy storage device, is a marginally stable system and that the health subsystem outputs do not affect the battery charge/discharge states instantaneously. The Two Step Filter can estimate both the state error and subsystem parameter successfully and thus provides the estimation with robustness against initialization errors. • Used linear examples to demonstrate the effectiveness of the Two Step Filter.
Industry Collaboration	None.
US-China Collaboration Activities	We have been engaged in research discussion with Professor Yang Geng's group in Tsinghua University, Beijing, China.
Issues of Concern	None.
Notable Recent Achievements	Zhou, X., Ersal, T., Stein, J. L., and Bernstein, D. S., 2014. “Battery State of Health Monitoring by Side Reaction Current Density Estimation via Retrospective-Cost Subsystem Identification”. ASME Annual Dynamic Systems and Control Conference, accepted.

Thrust Area 4: Advanced Lightweight Materials and Structures

Thrust	TA 4: Advanced Lightweight Materials and Structures
Title	**Project 2: Cost effective lightweight materials (US Cooperative)**
Personnel	PIs: Prof. Jose M. Castro (OSU), Glenn Daehn (OSU) Graduate students: Ziwei Zhao (OSU)
Objective	To develop cost-effective light weight structures for next generation vehicle. Key barrier is the balance of processability and performance of the new composites. Our project focuses on developing nano-enhanced Fiber reinforced Polymeric Composites (FRPCs) with adequate processability. One method to do so is to locate a CNF nanopaper on the surface of glass fiber in the composites in order to provide surface conductivity and abrasion protection.
Progress Report	In the past three months, a series experiments were conducted in order to investigate the improvement of using nanopaper on the surface of fiber reinforced polymeric composites. We have demonstrated that CNF-PANI nanopaper enhanced composites have a larger elongation to break than conventional composites. CNF-Acid nanopaper does not provide much improvement because acid treatment shortens CNF particles. CNF-Acid treated nanopaper is not as strong as CNF-PANI nanopaper. We applied CNF-PANI nanopaper to different types of glass fiber mats. The one we used before is thin and strong. In general, the elongation to break is increased with the use of nanopaper. For the bidirectional glass mat, Windstrand, the maximum flexural strength can be increased from 150MPa to about 200 MPa.
Industry Collaboration	• Nano Materials Innovation, a spinoff company from OSU, collaborates in the surface modification of nanoparticles.
US-China Collaboration Activities	Describe interactions with Chinese partners for this period of performance. • None
Issues of Concern	• The permeability of the nanopaper is low, making the impregnation difficult. This has the potential of slowing down the process of composites fabrication. • The dimension of nanopaper is currently limited. Fabrication process is slow. Currently working in addressing both concerns
Notable Recent Achievements	Describe any product produced or tech transfer activity such as: • Permeability Measurements and Flow Simulation for Polyaniline (PANI) Carbon Nano Fibers (CNF) Modified Nanopaper on Glass Fiber Preform, Polymer Composites, 2014. • Ziwei Zhao, Wei-Ching Liao, L. James Lee, Jose M. Castro. "Permeability analysis of carbon nanofiber nanopapers." 30th International Conference of the Polymer Processing Society, 2014. • Wei-Ching Liao, Eusebio D. Cabrera, Ziwei Zhao, Ying-Chieh Yen, Jiangfeng Yu, Jose M. Castro, L. James, Lee. "Simulation of nanopaper permeability and injection molding using smoothed particle hydrodynamics." 30th International Conference of the Polymer Processing Society, 2014.

Thrust	4: Advanced Lightweight Materials and Structures
Title	**Project 3.2: Joining in Multi-Material Structures**
Personnel	Prof: Glenn S. Daehn Student: Steven Hansen, The Ohio State University
Objective	• Recently, we have developed a technique that appears capable of producing solid-state impact welds between arbitrary pairs of dissimilar metals in a manner analogous to explosive welding. This newly developed method creates a pressure pulse by vaporizing a thin metal foil using a pulsed electrical current. While very large and thick plates are joined in explosive welding, our method has proven applicable for the sizes of material relevant to automotive construction, being able to accelerate mm-scale sheet metal to over 1 km/s within a few mm. • Work to understand and characterize the vaporizing foil actuator (VFA) launch is continuing. Next steps include parameter variation experiments with previously unused flyer variants, as well as improvement of an analytical model employing the Gurney velocity of the expanding foil vapor. • We are now investigating longer continuous sheet-to-sheet solid-state welds using a newly built vaporizing foil actuator metalworking fixture, which is capable of handling workpieces three times longer than the old setup - an active working region of up to 9 inches.
Progress Report	• Additional experiments varying input electrical energy and vaporizing actuator thickness have been completed using Cu110 and CP Ti flyers at ~0.5 mm thick. Analysis of the recorded current, voltage, and velocity traces shows that the relationship between average driving pressure and energy deposited into the vaporizing actuator (normalized between the various foils by their energy for vaporization) is linear, as expected. • Initial experiments with the new VFA fixture have produced successful solid-state welds greater than 4” long between ~0.5 mm thick AA6061 T6 sheets.
Industry Collaboration	**Describe interactions with industry partners for this period of performance (see metrics in China collaboration section)** • No significant interactions this period.
US-China Collaboration Activities	**Describe interactions with Chinese partners for this period of performance.** • No significant interactions this period.
Issues of Concern	**Describe any barriers to achieve objectives** • No significant barriers this period.

Notable Recent Achievements	**Published:** • A. Vivek, S.R. Hansen, and G.S. Daehn, "High strain rate metalworking with vaporizing foil actuator: Control of flyer velocity by varying input energy and foil thickness," *Review of Scientific Instruments*, **85**, 075101-1, 8 (2014). • A. Vivek, R.C. Brune, S.R. Hansen, G.S. Daehn, "Vaporizing foil actuator used for impulse forming and embossing of titanium and aluminum alloys," *Journal of Materials Processing Technology*, 214, 865-875, 2014. **Accepted conference papers:** • S.R. Hansen, A. Vivek, and G.S. Daehn, "Control of Velocity, Driving Pressure, and Planarity in Flyer Launch with Vaporizing Foil Actuator," submitted to 6th International Conference on High Speed Forming, Daejon Korea, April 2014. • S.R. Hansen, A. Vivek, and G.S. Daehn, "Vaporizing Foil Actuator: Controlling the Pressure Pulse for Impulse Metalworking," submitted to Proceedings of the 2014 ASME Manufacturing Science and Engineering Conference, University of Michigan, USA, June 9-13, 2014.

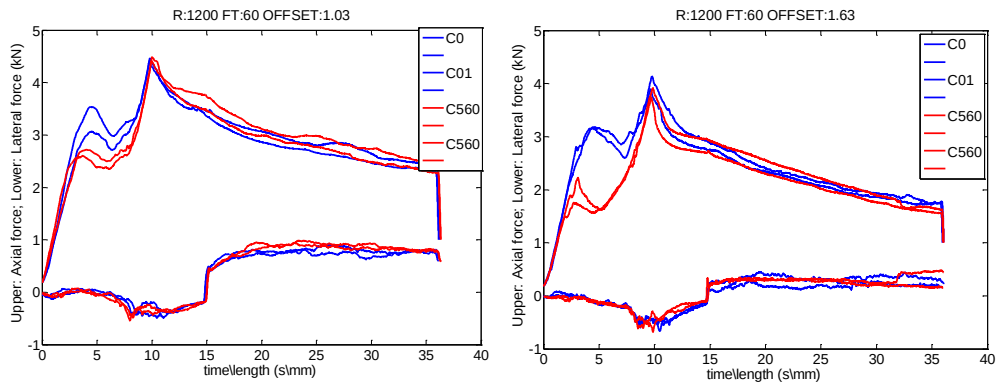
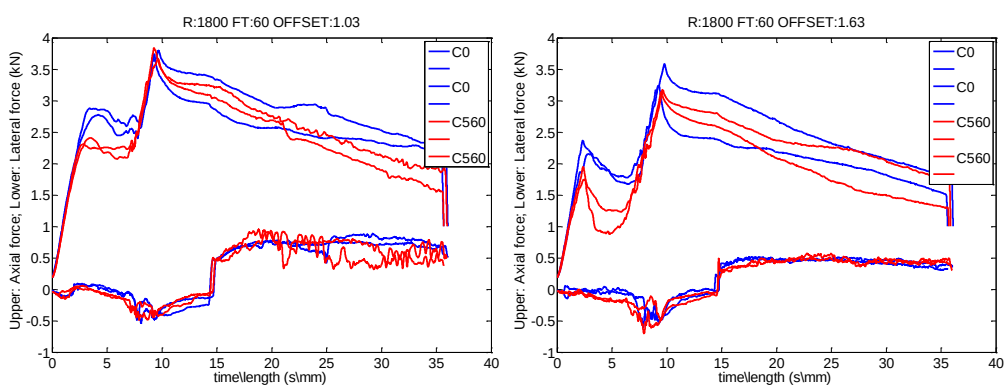
Thrust	TA 4: Advanced Lightweight Materials and Structures
Title	**Project 3: Joining multi-material vehicle structures (Joint)**
Personnel	PI: Jun Ni (UM) Post Doctor: Shuhuai Lan (UM) Graduate student: Xun Liu (UM)
Objective	• Develop high-quality and economical joining processes between dissimilar lightweight materials.
Progress Report	Effects of the electrical current under different process conditions were experimentally studied. Based on our previous results of friction stir welding of dissimilar aluminum alloy 6061 and advanced high strength steel TRIP 780/800, welding speed has an insignificant effect on the mechanical welding force. Accordingly, only rotational speed and tool offset were varied in our experiments while welding speed was selected to be 60mm/min. Tool offset is defined as the distance between tool axis and the faying surface of the two materials. Larger tool offset means the tool is shifted more into aluminum alloy.  Fig. 1 Effects of tool offset under rotational speed of 1200 rpm Fig. 1 shows the effects of different tool offsets under rotational speed of 1200 rpm. Blue lines correspond to the conditions where no current was applied while red lines show the force results under electrically assisted scenarios. It can be seen that the applied current can effectively reduce the axial force during plunge stage. However, electricity can hardly affect the force during the welding stage, including both the axial force and lateral moving force. Moreover, the force reduction is more significant under a larger tool offset, which is due to the relative configuration of the electrodes in our experiments. Similar results can also be observed in Fig. 2, where a larger value of rotational speed was applied. 

Fig. 2 Effects of tool offset under rotational speed of 1800 rpm

In order to further consider the thermal effects due to resistance heating, temperature was measured during the process. Three thermocouples were buried along the weldline in the backing plate and the experimental configuration is shown in Fig. 3. However, in order to guarantee the electrical insulation between the workpiece and backing plate, thin mica sheet needs to be inserted. The mica sheet, on the other hand, will insulate the heat as well. The measured temperature results were shown in Fig. 4. It can be observed that good consistency can be achieved but the highest temperature is less than 100°C.

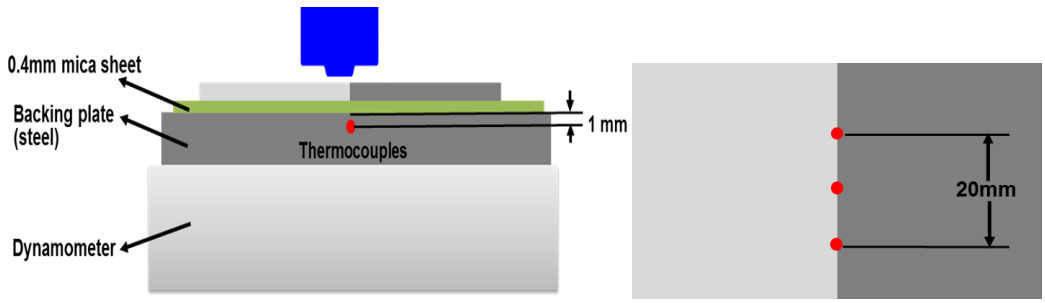


Fig. 3 Experimental configuration for temperature measurement during the hybrid FSW process

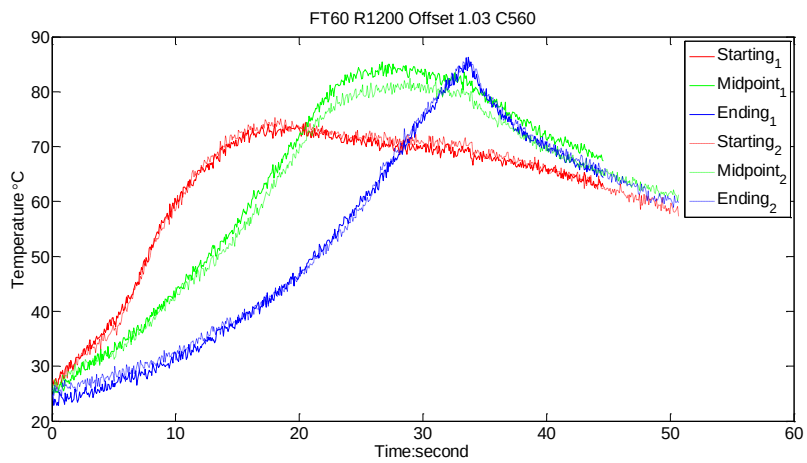
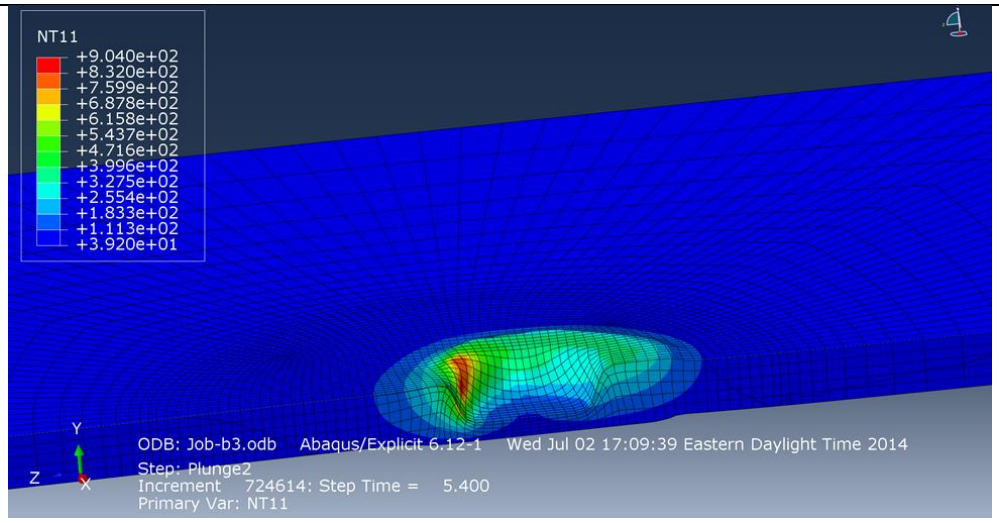
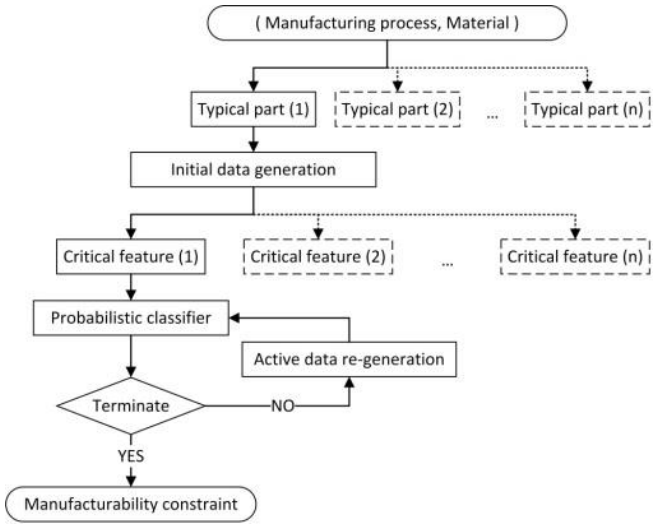
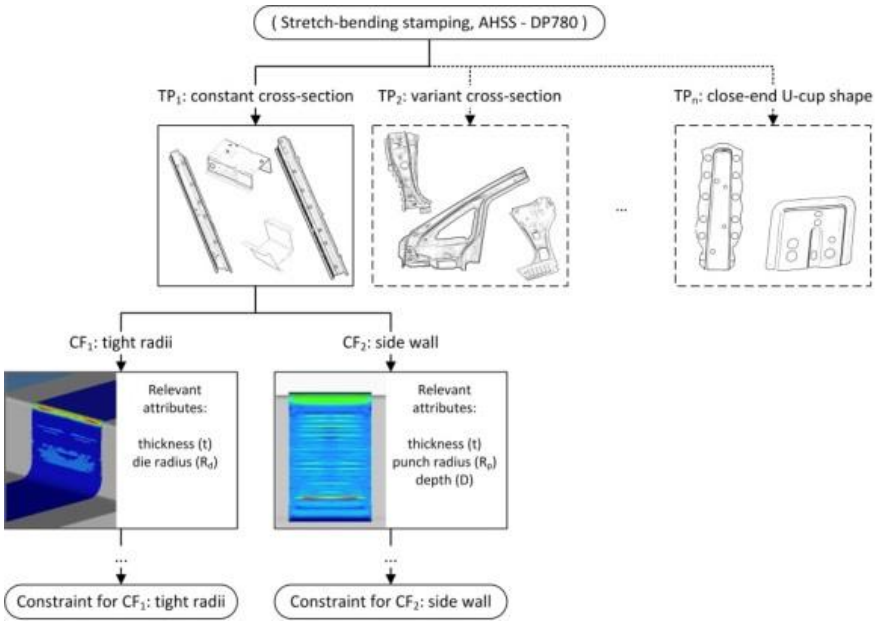


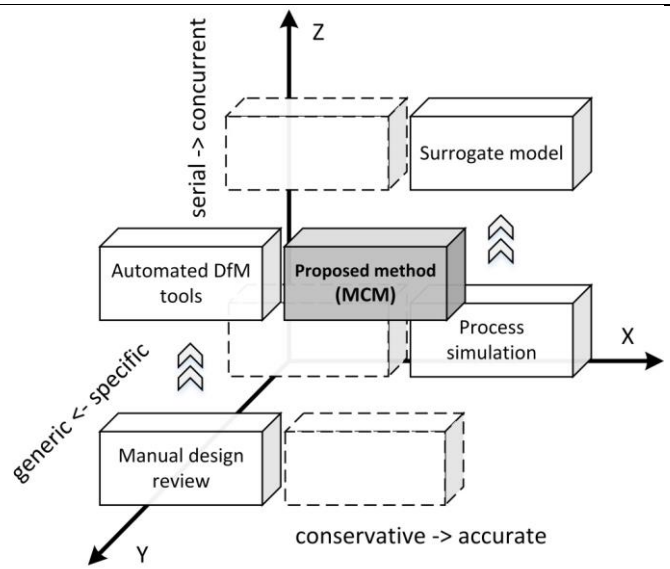
Fig. 4 Temperature measurement results

A finite element analysis model based on the commercial FEA software Abaqus has been developed for the plunge stage of the dissimilar friction stir welding process. Due to the great element distortion during this stage, the ALE (Arbitrary Lagrangian-Eulerian) needs to be applied during the calculation. However, the Abaqus software could not perform ALE on different materials and extremely distorted elements can be observed on the boundary of the two materials, which will lead to abortion of the program. In order to account for that, a subroutine has been written for considering the two material properties and the temperature results predicted by the developed model can be shown in Fig. 5.

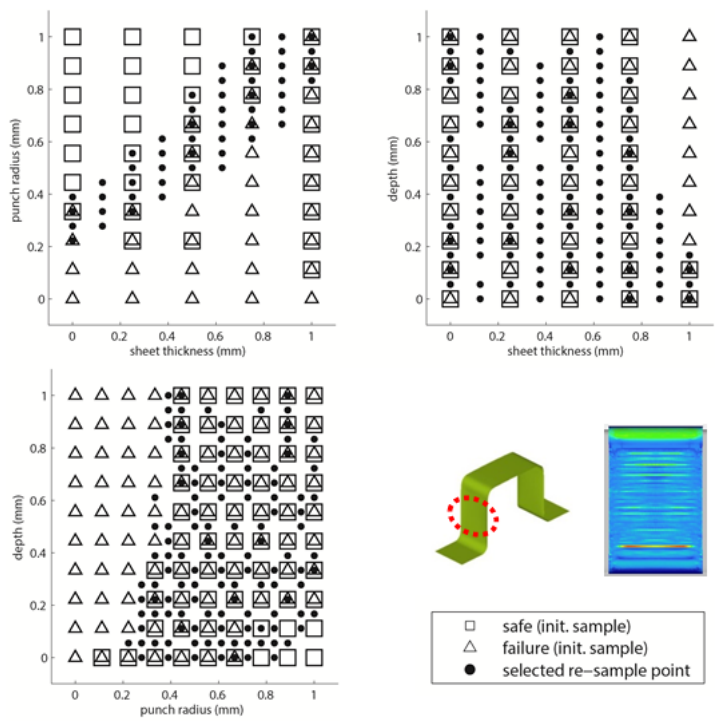
	 Fig.5 Temperature distribution during plunge stage calculated by the developed FEA model based on Abaqus
Industry Collaboration	• N/A
US-China Collaboration Activities	• N/A
Issues of Concern	• Improvement should be made on temperature measurement in the experimental setup
Notable Recent Achievements	• Patent 2115-005675-US-PS1, Hybrid Friction Stir Welding for Dissimilar Materials Through Electro-Plastic Effect, Xun Liu, Shuhuai Lan, Jun Ni, referenced provisional patent application filed

Thrust	TA 4: Advanced Lightweight materials and structures
Title	**Project 4: Hybrid materials Interface Increased Strength method and modeling Cooperative (US)**
Personnel	PIs: M. D. Thouless (UM) Graduate students: James Gorman (UM)
Objective	To demonstrate a methodology for modeling the bonding of hybrid materials, such as composites and metals with a focus on demonstrating its capability for design and to capture the effects of surface modification. To work with industry to implement an approach to evaluate and design hybrid joints for light-weight materials. • No change
Progress Report	We have developed a mode-II test specimen. Initial experiments indicated that it might be difficult to make specimens large enough to use a *J*-integral approach. Subsequent experiments indicated that it should be possible to use a specimen with a short ligament to measure the mode-II traction-separation law directly. Mode-II specimen (lap-shear geometry) with short ligaments have been made and tested. Digital image correlation (DIC) techniques have been used to measure the shear displacements along the interface. These have confirmed that the displacements are uniform and can be used directly to determine the shear-traction law. The mode-II strength is 24 ± 2 MPa, and the mode-II toughness is 1400 ± 500 J/m^2
Industry Collaboration	• Regular conference calls with Eaton • New production adhesive selected by Eaton; testing will commence once experimental procedure is finalized.
US-China Collaboration Activities	• NA
Issues of Concern	The variation in the critical displacement for the shear is rather. The reason for this is not understood, and needs further work.
Notable Recent Achievements	

Thrust	TA 4: Advanced Lightweight Materials and Structures
Title	**Project 4: Multi-Material Lightweight body subsystem & vehicle optimization (Joint)**
Personnel	PIs: Kazuhiro Saitou (UM), Qing Zhou (THU), Dafeng Jin (THU), Xinmin Lai (SJTU), Zhigang Yang (Tongji) Faculty participants: Liang Tang (THU), Yongbing Li (SJTU) Graduate students: Yuqing Zhou (UM), Zhongqi Yu (SJTU), Hua Wang (SJTU)
Objective	Develop a methodology for economically integrating components made of lightweight materials (Al, Mg, HSS/UHSS) in vehicle body structure with maximum weight reduction benefit
Progress Report	Note: Due to the discontinuation of funding in Chinese CERC, there is no activity by Chinese partners during this quarter. • Refined the overall method flow for manufacturability constraint modeling (MCM) (above figure) and example flow on AHSS stamping (below figure);   • Summarized the originality claim for MCM compared with existed DfM solutions;



- Identified the *critical feature: side wall* for AHSS stretch-bending process, selected relevant geometric attributes and constructed the manufacturability constraint. The data mining result showed difference with published empirical design guidelines which we considered as hidden knowledge that is hard to be captured empirically yet can be mined by MCM;



- Started extending MCM to cost-based manufacturing constraint modeling on lightweight composite molding process.

Industry Collaboration	• Attended BASF-UM networking event in Ann Arbor, gave an oral presentation and presented a poster on MCM.
US-China Collaboration Activities	• Continued to interact with SJTU team to compile DFM constraints for HSS/AHSS stamping. Further experiment on material constant calibration for shear fracture failure criteria might be conducted by SJTU team.

Issues of Concern	• The year 4 and 5 continuation of Chinese CERC.
Notable Recent Achievements	• Summarized current result on MCM and finished a manuscript to be submitted to a journal publication.

Thrust Area 5: Vehicle Grid Integration

Thrust	TA 5: Vehicle Grid Integration
Title	**Project 2: Vehicle-Grid System modeling for technology deployment (Joint)**
Personnel	PIs: Ramteen Sioshansi (OSU), Songbin Sun (THU) Graduate students: Fei Wu, Xiaoli Liu (OSU)
Objective	• Assess grid impacts of large-scale deployment of PEVs • Develop a technology roadmap and policy recommendations for accelerating electric vehicle deployment in the U.S. and China
Progress Report	• Paper focusing on numerical case studies demonstrating benefits of controlled PEV charging on reducing wind-uncertainty costs under revision for publication in *Energy* • Invited paper on synergies between PEV charging and integration of renewable energy sources into electric power systems submitted for publication in *Revue d'Économie Industrielle* • Preparing paper on spatial effects on PEV adoption within the state of Ohio for publication in *Spatial Economic Analysis* • Beginning more spatially detailed modeling of central Ohio at the street level • Received research grant from Google to geocode central Ohio vehicle registration data • Determining optimal charging station locations in northeastern Ohio based on interested from FirstEnergy (an industrial partner) • Preliminary work examining distribution-level effects of level-3 fast PEV charging stations • Modeling effects of level-3 fast PEV charging stations co-located with big-box retailers on aging of existing transformers • Developing structure for stochastic dynamic programming model to use distributed generation and energy storage to relieve transformer loading due to level-3 fast PEV charging
Industry Collaboration	• AEP and FirstEnergy are active industry partners, with regular input on research being provided at semi-annual SMART@CAR meetings at The Ohio State University's Center for Automotive Research • AEP and FirstEnergy are actively involved in helping to explore power system and distribution-level effects of level-3 charging • Conducting an analysis of optimal charging station locations in northeast Ohio based on interest from FirstEnergy • AEP providing load and transformer rating data for level-3 charging station modeling • Eaton has expressed interest in charging infrastructure design optimization model, and we are engaged in discussions with them centering around the EVTown project
US-China Collaboration Activities	• Monthly webinars with Chinese counterparts continue to further establish joint research
Issues of Concern	n/a
Notable Recent Achievements	• X. Xi and R. Sioshansi, "Wind Integration Benefits of Plug-in Electric Vehicles," under revision for publication in *Energy* • C. Weiller and R. Sioshansi, "The Role of Plug-In Electric Vehicles with Renewable Resources in Electricity Systems," submitted to *Revue d'Économie Industrielle*

Thrust	TA 5: Vehicle-Grid Integration
Title	**Project 4: Control strategies for vehicle-grid integration (Cooperative)**
Personnel	PI: Ian Hiskens (UM), Hongbin Sun (TU), Qinglai Guo (TU) Graduate students: Ian Beil (UM)
Objective	Develop control strategies that mitigate distribution-level issues associated with high penetrations of PEVs, and that allow PEVs to provide operational services to the wider grid.
Progress Report	• Developed large-scale PEV model that emulates the behavior of significant vehicle penetration levels on the power system load profile • Rigorously defined previously developed control theory to show situations in which both large-scale and local control are simultaneously possible • Currently extending this theory to define optimal charging strategy in the presence of limited communication capabilities
Industry Collaboration	
US-China Collaboration Activities	• Participated in web-based meetings with US and Chinese collaborators.
Issues of Concern	
Notable Recent Achievements	• Paper accepted: "Coordinated PEV Charging and its Effect on Distribution Network," to be presented at the Power Systems Computation Conference in Wroclaw, Poland August 18-22, 2014

Thrust	TA 5: Vehicle Electrification
Title	**Project 4: A Wireless Magnetic-Resonance Power Transmission System for EV Charging (US Cooperative)**
Personnel	PI: Chris Mi (UM-Dearborn) Post-doctors: Zhang Wei (Joined the project on March 1, 2014) Hijie Zhou, Post-Doctor Graduate students: Fei Lu (UM-Ann Arbor) Tianze Kan (UM-Dearborn) Visiting scholar: Weihan Li (Hefei Univ. of Technology), Junjun Deng (Northwestern Polytechnical Univ.) (PhD Student)
Objective	• Analyze the resonant condition or near-resonant condition (frequency bandwidth). Perform theoretical analysis of maximum power transfer and maximum efficiency between the transmitter and the receiver, detailing the requirements and constraints of distance, power, geometry, and lateral and angular misalignments. • Develop analytical methods based on S parameters (including the Smith-chart) for the two-port network to calculate the key parameters, such as the maximum efficiency, the coupling coefficient, the power quality factor Q, the coil's self-inductance and mutual-inductance, the radiation resistance and the Ohmic resistance. • Develop an analytical model based on C++ or Matlab and numerical models based on finite-element method (FEM) to verify the correctness of the proposed methods. • Perform analytical analysis on the effects of a finite, conducting body on the charger. Perform FEM simulations in the presence of finite conducting bodies to verify the analysis and explore more complex geometries found in an automotive environment. • Construct the coils based on the analytical analysis and simulation results, and design the control and energy conversion systems. Develop a hardware prototype with corresponding co-FEM simulation model to verify the key aspects of the analysis. • Build a hardware prototype for placement in an automotive environment to test the performance. • Develop an algorithm for object detection between the source and the receiver coils for practical study. • Evaluate the magnetic field levels using published *IEEE/SAE* standards as a function of frequency and its impact on human body.
Progress Report	• Study litz wire replacement • Study pad size reduction • Compare different coil structures: circular, DDQ, bi-polar, flux tunnel • Compare different compensation topologies and their effectiveness with focus on compensating leakage or self-inductance • Develop, design, and test, AC-Battery system including rectifier, PFC, and DC-DC, incorporation with LCC compensation topology of the wireless portion of the system; 6.7kW power and 93% efficiency is achieved • Studied the parameter sensitivity of the LCC topology • Studied the interaction of auxiliary coil in the double sided LCC topology
Industry Collaboration	• Working with DENSO on the demonstration of a prototype onto a production car • Gained help from Underwriters Laboratories (UL), Dr. Hai Jiang from UL helps with coil design and optimizations
US-China Collaboration Activities	• IP disclosures filed; US, China, filed; and international patents planned • Commercialization of CERC-CVC IP by Mia Motors, and DENSO • Proposed a special issue for the IEEE Transactions on Power Electronics, Special Issue on Wireless Power Transfer (EIC: Chris MI) with a due date on October 31; both China and US partners are encouraged to submit papers

	• Managed a special issue for the IEEE Journal of Emerging and Selected Topics in Power Electronics, Special Issue on Wireless Power Transfer (EIC: Chris MI). Both China and US partners have submitted papers and accepted by this special issue • Had many technical discussion with John Miller of ORNL • One Post-doctoral fellows trained • Delivered a tutorial on wireless power transfer for the IEEE Applied Power Electronics Conference (conference has 4500 attendees) in March 2014 • Invited to deliver a tutorial on wireless power transfer at the ITEC (International Transportation Electrification Conference – Asia Pacific), Beijing, August 31, 2014. • Invited to deliver a e-learning module for IEEE Future Directions Committee, to be recorded and • Chris Mi was appointed as the General Co-Chair of IEEE Workshop on wireless power transfer 2015; sponsored by six IEEE societies (PELS, IAS, IES, MAG, PES, VTS, and KAIST) • Worked with ANSYS to develop a workshop on wireless power transfer on March 13, 2014 at the University of Michigan-Dearborn.
Issues of Concern	• How to protect IPs • How to further the technology development • How to commercialize the technology with OEM and supplier, CERC partners • Additional funding support for further development and commercialization of the technology
Notable Recent Achievements	• Presented one paper at the IEEE APEC March 2014; • One paper accepted by IEEE Transactions on Vehicular Technology • One paper accepted by IEEE Journal of Emerging and Selected Topics in Power Electronics, Special Issue on Wireless Power Transfer • Filed three patent in US and two patents in China; world patent rights are planned. • Worked closely with DENSO International on the commercialization of the IPs. • Worked closely with KAIST (Korean Advanced Institute for Science and Technology). KAIST is one of the first organizations to build power roadways with wireless power transfer technology. • Two more papers submitted to APEC 2015 • One paper accepted by IEEE Trans. On Industrial Electronics with revisions.

Thrust	TA 6: Energy Systems Analysis, Technology Roadmaps
Title	**Project 1: Life Cycle Assessment of Wireless Charging of Electric Vehicles (Collaboration Status: Joint)**
Personnel	PI: Gregory Keoleian (UM) Research Specialist: Robb De Kleine (UM) Graduate students: Zicheng (Kevin) Bi (UM) Visiting scholar: Lingjun Song (Beihang University, China)
Objective	• Compare the environmental performance of wireless charging to plug-in charging for electric vehicles using life cycle assessment • Conduct life cycle inventory analysis of both wired and wireless charging hardware • Develop a model to assess the energy, environmental and economic performance of wireless charging including potential lightweighting benefits from battery size reduction for fixed route vehicles such as transit buses
Progress Report	*April 2014* • Prepared figures, tables and presentation slides of preliminary findings *May 2014* • Presented the preliminary findings at the CERC meeting on May 2, 2014 and got feedbacks from industrial partners including Denso and Delphi • Refined the model structure and key parameters, such as charging efficiency and lightweighting correlation, based on presentation feedback • Began to draft a paper for publication *June 2014* • Presented a poster and won the third place at the BASF-University of Michigan poster presentation on June 26, 2014, sharing research findings on the topic of "energy storage devices and materials" and highlighting our battery downsizing model for wireless charging electric buses • Revised the plug-in charger inventory by tearing down a sample charger provided by Delphi • Finished an initial draft of the paper
Industry Collaboration	• Peter Hoffman at Delphi Automotive provided a plug-in charger for teardown and analysis • Significant feedback on analysis provided by partners at Delphi and Denso at the CERC meeting on May 2, 2014
US-China Collaboration Activities	• Co-author of a paper in preparation: Lingjun Song (visiting scholar from School of Transportation Science and Engineering, Beihang University, China)
Issues of Concern	• None this quarter

Notable Recent Achievements	• Received the Outstanding Presentation Award and won the third place at the BASF-University of Michigan poster presentation on June 26, 2014
	• Publications:
	  ○ Lewis, A.M., J.C. Kelly, G.A. Keoleian. Vehicle lightweighting vs. electrification: Life cycle energy and GHG emissions results for diverse powertrain vehicles. *Applied Energy* (2014) 126: 13–20.
	  ○ Lewis, A., Keoleian, G., and Kelly, J., "The Potential of Lightweight Materials and Advanced Combustion Engines to Reduce Life Cycle

	Energy and Greenhouse Gas Emissions," *SAE Technical Paper* 2014-01-1963, 2014, doi:10.4271/2014-01-1963. • Presentations: ○ "The Impact of the Grid on Vehicle Life Cycle Sustainability" Steel Market Development Institute, Livonia, MI, May 14, 2014. • "Reducing GHG Emissions from Vehicle Lightweighting and Electrification? The power of the grid." Emissions 2014, Global Automotive Management Council Conference, June 11, 2014.

Thrust	TA 6: Energy Systems Analysis, Technology Roadmapping, and Policy
Title	**Project 2: Parametric Analysis of Clean Vehicle and Fuel Deployment in the Light Duty Transportation Sector (US Cooperative)**
Personnel	PIs: Dawn Manley (SNL), Todd West (SNL), Garrett Barter (SNL)
Objective	• Parametric analysis of the feasibility of and opportunities for large-scale penetration of clean vehicle and fuel technologies in the light duty transportation sector.
Progress Report	• Completed analyses that consider impact of range penalties, infrastructure availability, and recharge time on BEV adoption using driving distributions that represent real world data. The model considers the difference in adoption based on representing penalties as a cost associated with these factors versus thresholds for frequency of inconvenience for insufficient range. Analyses show willingness to adopt EVs varies based on battery range and driver characteristics. Drafted manuscript that is under review by CERC industrial collaborator.
Industry Collaboration	• Industry partner instrumental in project scoping, assumptions, and assessment of results.
US-China Collaboration Activities	
Issues of Concern	• None
Notable Recent Achievements	• Drafted manuscript that is under review by CERC industrial collaborator.

Thrust	Thrust 6: Energy Systems Analysis
Title	**Project 2.2: Fuel mix strategies and constraints (Collaboration Status: Cooperative US)**
Personnel	PI: Ming Xu (UM) Graduate Student: Hua Cai, Tricia Pontau (UM)
Objective	• The objective of this project is to assess the feasibility of alternative vehicle fueling including biofuels and electricity for meeting significant penetration of clean vehicles. This project will highlight critical resource availability and infrastructure constraints for both biofuels and electricity generation. This project will be complemented by activities that will address grid control and resilience in Thrust 6.
Progress Report	April: Conducted state level land demand assessment of both biological systems (switchgrass ethanol, corn starch ethanol, and open pond algae biodiesel) and engineered systems (electricity generated from wind, electricity generated from solar, closed system algae biodiesel). Updated solar calculation. May: Presented paper titled "Informing Electric Vehicle Public Charging Infrastructure Development using Travel Patterns Mined from Big-Data" in 2014 International Symposium on Sustainable Systems and Technology (ISSST) held in Oakland, California and was awarded 3rd Place for Student Paper Competition. June: Finishing manuscript entitled "Assessing Land Use Impact by Clean Vehicle Systems" to be submitted to journal Resource, Conservation and Recycling in July.
Industry Collaboration	• In contact with Microsoft for potential collaborations
US-China Collaboration Activities	• Attended and presented at TA6 CERC Web-Ex Meetings
Issues of Concern	None to date
Notable Recent Achievements	• Manuscript titled "Assessing Land Use Impact by Clean Vehicle Systems" prepared for journal submission. • Conference paper titled "Informing Electric Vehicle Public Charging Infrastructure Development using Travel Patterns Mined from Big-Data" awarded 3rd Place Student Paper in 2014 International Symposium on Sustainable Systems and Technology (ISSST) held in Oakland, California.

Thrust	TA 6: Energy Systems Analysis, Technology Roadmaps & Policy
Title	**Project 4: Clean Vehicle Technology Roadmap & Policy Recommendations: Task 4.1 – 4.5 Fleet Modeling on China's Alternative Fuels. (US Cooperative)**
Personnel	PIs: John Heywood (MIT) Graduate student: Summer Jiakun Zhao (MIT)
Objective	• Present the differences of future vehicle stock, fuel consumptions, and CO2 emissions from models including FLEET (MIT), EPPA (Emissions Prediction and Policy Analysis, MIT), and TCAEM (Tsinghua China Automotive Energy Model). • Project the growth, energy consumption, and CO2 emissions of electrified vehicles, including BEV, HEV and PHEV in China for the next 35 years. • Forecast the electric utility capacity expansion and the energy mix in China for the next 35 years. • Predict the amount of CO2 emissions and air pollution that can be reduced through the penetration of electrified vehicles, and map whether emissions would be distributed to rural areas instead.
Progress Report	• April: Communicated with professors from Tsinghua to obtain more detailed information and to update the comparison results; consolidated all the information together and started drafting the comparison paper. • May: Conducted a project that compared five vehicle technologies including BEV, HEV, PHEV, Ethanol (E85) and Methanol (M85) based on their cost/mile and CO2 emissions/mile. • June: Used the FLEET model to explore the electrified vehicle penetration and researched the potential electric utility capacity expansion model to be used for China.
Industry Collaboration	N/A
US-China Collaboration Activities	• Exchanged partial comparison results with professors in Tsinghua, and obtained more detailed data from them on their model results. • Discussed with the China Energy and Climate Project about the potential collaboration on researching the relationship between electrified vehicles and air pollutions in China.
Issues of Concern	Difficulties come into modeling the electric utility capacity expansion in China, and decision has to be made on whether spending time to build my own model or using existing models; also has to decide the level of focus, i.e. national level, city level, or several key cities.
Notable Recent Achievements	N/A

Thrust	Thrust 6. Energy Systems Analysis, Technology Roadmaps and Policy
Title	**Project 4. Clean Vehicle Technology Roadmap and Policy Recommendations**
Personnel	PI: John M. DeCicco (UM)
Objective	Evaluate and identify combinations of Clean Vehicle-Fuel System (CVFS) technologies and deployment rates for achieving national energy and GHG goals under varying assumptions regarding technology maturation and market growth. Develop new modeling tools as needed for this effort.
Progress Report	This quarter saw the near-completion of a major research effort of the past three years as part of CERC-CVC Thrust 6, Project 4. Building on previously reported results and after making revisions based on peer review comments, a new paper, "The Liquid Carbon Challenge: Evolving Views on Transportation Fuels and Climate" (citation below) was published online and is forthcoming in the journal. This work deconstructs established lifecycle-based Fuel Cycle Analysis (FCA) methods, as embodied in models such as GREET, that are widely used for clean vehicle technology roadmapping and policy analysis studies. Comparing FCA to other methods of carbon accounting reveals that, in addition to large and irreducible uncertainties, FCA has serious structural flaws including an incorrect carbon cycle representation, misspecified system boundaries and the inappropriate use of an equilibrium framework for a dynamic stock-and-flow problem. This analysis implies significant new research needs including, for example: • redesigning the core structure of FCA models and developing protocols for appropriated qualified reporting and application of FCA results; • empirically testing model assumptions about CO_2 uptake in biofuel feedstocks; • retrospectively evaluating the measurable GHG impacts of actual biofuel production to date in order to better calibrate the modeling used to project the prospective performance of future vehicle-fuel systems; • exploring the applicability of systems dynamics methods, which may be better suited to the stock-and-flow nature of biofuel vs. fossil fuel comparisons. These findings also suggest a need for better coordination across relevant research communities, such as between DOE's biofuels programs and programs in DOE's office of science that address terrestrial carbon cycle measurement and analysis.
Industry Collaboration	Although it did not involve direct industry collaboration, substantive comments were received from CERC industry partners and others in the auto and energy industries.
US-China Collaboration	No direct collaborations underway.
Issues of Concern	Because these new findings challenge established vehicle-fuel systems analysis methods widely used by CERC-CVC partners as well as by other researchers and policymakers, further vetting and discussion are warranted.
Notable Recent Achievements	Publication of "The liquid carbon challenge: evolving views on transportation fuels and climate" by J.M. DeCicco in *WIREs Energy & Environment*; the online preprint was posted 8 July 2014. doi:10.1002/wene.133

Thrust	TA 6: Energy Systems Analysis, Technology Roadmaps
Title	**Project 5: Assessment of automotive aluminum recycling infrastructure and allocation methods (Collaboration Status: US Cooperative)**
Personnel	PIs: Gregory Keoleian (UM) Research Specialist: Robert De. Kleine (UM) Graduate student: Arman (Mohammad) Golrokhian (UM)
Objective	• To evaluate the importance of material recycling on life cycle results based on characterization methods for energy consumption, global warming potential, and resource depletion. • To assess the outcomes of *Recycled Content* and *End-of-Life Recycling* methods in accounting for the effectiveness of lightweighting in improving environmental quality. • To compare the existing resource depletion characterization methods to identify the strength and weaknesses of each method, and to explore new approaches to better capture material scarcity in the context of automobile manufacturing. • To evaluate the effect of vehicle lightweighting using aluminum on energy, GHG emissions, and depletion of resources.
Progress Report	• Literature review has been conducted to identify existing resource depletion methods • Strengths, weaknesses, and gaps in existing resource depletion methods were identified • A preliminary model, which seeks to improve upon existing resource depletion methods, was initiated. The model considers material recycling, which is not included in existing models.
Industry Collaboration	• May 13, 2014: Participated in a meeting with steel and auto industry representatives and discussed recycling allocation approaches, and their relevance to transportation policy.
US-China Collaboration Activities	• Not at this time
Issues of Concern	• None at this time
Notable Recent Achievements	• Researchers were invited to prepare a proposal to the Steel Market Development Institute outlining further research exploring recycling allocation methods following the meeting on May 13, 2014. A proposal was submitted on June 13, 2014.