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. During the last quarter, each one of the US based tasks outlined implementation pathways which were reviewed by industry partners. These pathways highlight the commercialization potential of each project and the barriers for achieving the next steps in the TRL progression.

During the Industrial Advisory Board meeting in February, the implementation pathways were reviewed and a number of the projects, listed in the table below, were selected for closer collaboration between the researchers and the industry partners. A number of the industry partners are in discussion with the respective researchers to establish closer collaboration, and a few examples of these discussions are outlined in the collaboration section.

Thrust	Project	Task	Title	Industry Partner				
1	1	3	Li-ion battery aging and internal degradation mechanisms	Ford				
1	1	4	Perfromance and reliability of large format Li-Ion batteries					Honda
1	2	1	High Energy Density Battery Chemistries		Denso			
3	3	1	Rapid system integration through modular configuration, sizing and control	Ford	Denso	Eaton		
3	3	2	Intelligent Fault Diagnosis and Prognosis				Delphi	
3	4	1	Adaptive battery management system on and off the grid				Delphi	
3	4	2	Data-Based Techniques for Battery-Health Prediction				Delphi	
4	3	3	Friction Stir Welding of Dissimilar Metals				Delphi	
5	2		Vehicle-Grid System modeling for technology deployment		Denso			
5	3		Control strategies for vehicle-grid integration			Eaton		
5	4		A Wireless Magnetic-Resonance Power Transmission System for EV Charging		Denso	Eaton	Delphi	
6	5		Electricity and material sourcing scenario analyses to guide vehicle technology strategies	Ford				

Collaboration

- Monthly Thrust Area Web Ex meetings are running regularly and have been scheduled midway through 2014
- During the Society of Automotive Engineering Annual Congress, representatives from Delphi held a workshop with CERC-CVC researchers focused on Intelligent Fault Diagnosis and Prognosis. The session included discussions of pathways to commercialization for CERC-CVC research.
- Denso representatives discussed commercialization opportunities for wireless charging with CERC-CVC researchers.
- Delphi representatives also discussed commercialization opportunities for friction stir welding of dissimilar metals with CERC-CVC researchers.

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. Cost share spending will increase in the next 9 months to support a battery prototyping and characterization facility at the University of Michigan Energy Institute in connection with the Michigan Economic Development Corporation and their contribution to the battery hub work performed by UM, as well as a research partnership with Ford Motor Company. As part of the cost share commitment from the University of Michigan, $750,000 is budgeted for equipment in this battery lab, which is expected to be operational by the end of 2014.

Budget Period 1 - 4	Budgeted	Actual
DOE	$ 8,515,180	$ 6,696,371
Cost-share	$ 17,012,837	$ 7,531,666
Total	$25,528,017	$14,228,037

Schedule Status

Detailed schedules were developed by the US and Chinese researchers and were reported in the Joint Work Plan. Projects are now on track with a 6 month shift of timing due to the delays in contracting.

Publications / Key Outcomes / Awards

Awards received

- The paper published by 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" in 2013 American Control Conference was selected to receive the Best Paper Award by ASME Automotive and Transportation Systems Technical Committee.

Advanced Batteries and Energy Conversion

Ramdon, S., and Bhushan, B. "Nanomechanical Characterization and Mechanical Integrity of Unaged and Aged Li-ion Battery Cathodes," *J. Power Sources*, (accepted)

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," submitted to *Advanced materials*

Invited article in Journal of The Electrochemical Society's Focus Issue on Mathematical Modeling of Electrochemical Systems at Multiple Scales: Crystal Surface and State of Charge Dependencies of Electrolyte Decomposition on $LiMn_2O_4$ Cathode. Kumar, N.; Leung, K.; and Siegel, D. J. J. Electrochem. Soc. 2014 161(8): E3059-E3065; DOI:10.1149/2.009408jes

"DME decomposition on Li_2O_2 surfaces: Role of peroxide and superoxide terminations" for oral presentation at 248th ACS National Meeting (San Francisco, CA) in the Modeling and Simulations of Electrochemical Interfaces and Materials for Energy Storage (COMP division) symposium. (Submitted)

Kang, S.; Mo, Y.; Ong, S. P.; Ceder, G. (2014). "Nanoscale Stabilization of Sodium Oxides: Implications for Na-O2 Batteries." *Nano Letters* **14**(2): 1016-1020.

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

Report on cymene oxidation accepted for presentation to the 35th International Symposium on Combustion (to be held in August 2014)

Junfeng Zhao and Junmin Wang, "Adaptive Observer for Joint Estimation of Oxygen Fractions and Blend Level in Biodiesel Fueled Engines," IEEE Transactions on Control Systems Technology (in press), 2014.

Junfeng Zhao and Junmin Wang, "On-Board Fuel Property Identification Method Based on High-Pressure Common Rail Pressure Signal," ASME Transactions Journal of Dynamic Systems, Measurement, and Control, Vol. 136, No. 3, 031010 (9 pages), 2014.
Junfeng Zhao and Junmin Wang, "Engine Mass Airflow Sensor Fault Detection via an Adaptive Oxygen Fraction Observer," Proceedings of the 2014 American Control Conference (Invited Paper) (accepted), 2014.

Junfeng Zhao and Junmin Wang, "Engine onboard fuel property identification method using common rail pressure signal," Oct. 2012.

S. Hui, M. Nielson, D. Medlin, J. Salvador, J.P. Heremans, K.P. Pipe, and C. Uher, "Influence of Doping on the Thermoelectric Transport Properties in $CoSb_3$-based Skutterudites", accepted for publication *in Journal of Applied Physics*.

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*. DOI:10.1039/C4Cp00641K (2014).

Vehicle Electrification

Zhentong Liu, Qadeer Ahmed, Giorgio Rizzoni, and Hongwen He , *System Level Fault Detection and Isolation Scheme for Lithium-Ion Battery Pack*, submitted to CDC 2014

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*, submitted to DSCC 2014

Qi Chen, Qadeer Ahmed and Giorgio Rizzoni, *Sensor Placement Analysis For Fault Detectability And Isolability Of An Automated Manual* submitted to DSCC 2014

Jiyu Zhang, Andrea Cordoba-Arenas, Giorgio Rizzoni, *Fault Diagnosis for PMSM Drive System in Electric Vehicle*. Submitted to DSCC 2014

A paper on OCV model for SOC and SOH estimation was accepted and published on the Journal of Power Sources

Advanced Lightweight Materials and Structures

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.

S.R. Hansen, A. Vivek, G.S. Daehn, "Vaporizing foil actuator: controlling the pressure pulse for impulse metalworking," Proceedings of the 2014 ASME Manufacturing Science and Engineering Conference. (Accepted)

Liu, X., Lan, S., & Ni, J. (2014). Analysis of process parameters effects on friction stir welding of dissimilar aluminum alloy to advanced high strength steel. Materials & Design, 59, 50-62.

Liu, X., Lan, S., & Ni, J. (2014). Experimental study of electrically assisted friction stir welding of dissimilar Al 6061 to TRIP 780/800 steel, MSEC 2014, Detroit, Michigan, USA

Zhou, Y., and Saitou, K., "Identification of Manufacturability Constraints through Process Simulation and Data Mining", *Proceedings of the ASME 2014 International Design Engineering Technical Conference*, Buffalo, Aug 17-20, 2014, DETC2014-34542 (accepted)

Vehicle-Grid Integration

X. Xi and R. Sioshansi, "Wind Integration Benefits of Plug-in Electric Vehicles," submitted to *Energy*.

Energy Systems Analysis, Technology Roadmaps and Policy

None this period.

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 through in-situ characterization. In situ studies of a sealed electrochemical cell using the NIST Neutron Depth Profiling facility were performed during this quarter, showing the real-time evolution of the Lithium distribution. One task of the atomic scale modeling work is focusing on the decomposition of the organic electrolyte used in Li-air batteries. A deeper understanding of this process is critical as it is associated with undesirable phenomena such as capacity fade, high charging overpotentials, and limited cycle life. The atomic scale modeling is currently focusing on the difference in DME absorption between peroxide-like and superoxide-like surfaces of Li_2O_2, the primary discharge product in Li-O_2 batteries. Work also continues for the modeling of the properties of discharge phases in Na-O_2 batteries. At MIT, complementary work continues looking at the thermodynamic stability and the phase diagrams of various bulk sodium oxides.

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 investigation of 2,5-dimethylhexane, a key component of bisabolene, continued, with a specific focus on the high temperature decomposition of the fragment. All the reactions and their corresponding reaction rates were compiled into a sub-mechanism that describes the decomposition of the fuel and subsequent dissociation of the intermediates. This sub-mechanism was then incorporated into an existing "base mechanism" that describes the evolution of the system of smaller species created by our sub-mechanism. This new model that describes the evolution of 2,5-dimethylhexane was

used to simulate the behavior of the fuel in several situations, including shock tubes, rapid compression machines, and closed homogeneous reactors, bringing us one step closer to the goal of one model that will characterize a wide range of combustion temperatures and pressures. Powertrain efficiency gains post engine in the area of thermo electrics focused on studying transport measurements of newly fabricated Yb-filled and Sn-doped $CoSb_3$ samples.

In the electrification thrust, the finite element algorithm developed for electric machines are being optimized to improve simulation speed. By applying a polyphase time-periodic condition, the number of slip frequencies which can resonably be analyzed increases. Efforts continue to validate the approach by importing the models in commercial software and by comparing with results collected from hardware. Moving to the full-scale powertrain design, the systematic design procedure was extended from using two planetary gears to designs with multiple planetary gear and clutches. The algorithm now allows for efficient and systematic calculation of all possible configurations. After consulting with Ford researchers, an in-depth energy flow analysis was designed to better understand the source of improvement in energy consumption due to multiple-mode operations. The adaptive battery management system team was encouraged by the success on incremental capacity analysis based lithium ion battery state of health monitoring. The team is looking into the possibility of efficient multi-cell battery system identification using a similar modeling effort. A parametric battery model could be developed from single cell data and applied to other cells in the same pack, saving a significant amount of computational load, which is crucial for on-board 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. During this quarter, a series of experiments carried out to investigate the effect of spraying nanoparticles or using a nanopaper on the surface of a preform found that spraying about 5 weight percent of carbon nanotubes extended the elongation to break of the composite. The hybrid Friction Stir welding process incorporating electroplastic effects has been demonstrated on an adapted CNC machine and two types of electrode configurations have been investigated. Also, the electrical field distribution was studied using a finite element analysis software. At the vehicle level, researchers have proposed an active learning strategy for the sequential efficient design of experiments, drastically reducing the sampling computational cost. Also, parallel computing was used on process simulations and massive sampling which dramatically saved data generation time. In addition, the simulation tools were developed to accurately predict shear fracture for the high strength steel and ultra-high strength steel stretch-bending process.

Electrification is not just promising for increased efficiency; it also allows vehicles to interface with the electric grid and possibly renewable energy sources. The econometric modeling to study special effects on plug-in electric vehicles adoption within the state of Ohio is being finalized and refined to include spatial detail of central Ohio at the street level. In addition, modeling is being extended to examine distribution-level effects of level-3 fast charging stations. The research in thrust 6 also examined the ability of a large plug-in electric vehicle fleet to achieve large-scale electricity transmission objectives such as valley filling, demand dispatch, and

regulation while adhering to local distribution-level transformer overload and voltage quality constraints. A cohesive control strategy was developed that achieves higher level objectives without damaging the grid.

Finally, work continues in thrust area 6, the energy systems analysis, technology roadmaps, and policy thrust. The vehicle design and assessment work has completed the life cycle inventory of the material and manufacturing processes for a wireless charger and is progressing to the life cycle impact assessment of a wireless charger in terms of global warming potential and cumulative energy demand. The goal is to compare wireless and plug-in charging on a life cycle basis. With respect to alternative fuel vehicles, an initial analysis was completed that consider the impact of range penalties on battery electric vehicle drivers. The analyses show willingness to adopt EVs for a breadth of battery ranges and driver characteristics. The fuel mix strategy team finished a sensitive analysis for both biological systems and engineered systems to refine a regional optimal fueling strategy analysis. The research in to modeling of China's alternative fuels focused on the policies and current conditions of EVs, PHEVs, and HEVs, including policy targets, incentive programs, subsidies, barriers/challenges, charging infrastructures, consumer perceptions, and the involvement of state-owned enterprises.

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 (Joint)**
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: EELS has been carried out in the low energy-loss and core energy-loss (Li-k and Fe-M~55eV) regions on a standard $LiFePO_4$ nanoparticle (Sigma-Aldrich, > 97%) purity. Compositional inhomogeneity has been observed when these spectra are collected from three different regions of the same particle (Fig.1a). Li-K and Fe-M peaks appear or disappear and are shifted based on location within the particle. Similar inhomogeneity is observed by the study of the plasmon peak (23-24eV), which shifts based on location in the nanoparticle. Such compositional inhomogeneity has been previously recorded using x-ray diffraction (Fig. 1b). We plan to use the evolution of features in the low loss and core loss EELS spectrum with compositional homogeneity to study phases formed in the $LiFePO_4$ nanoparticle with cell aging. 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. <u>Standards Analysis:</u> 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. <u>In situ atomic force microscopy analysis of morphology and particle size changes in Lithium Iron Phosphate cathode during discharge</u>: In situ cell cycling data collected during AFM imaging is given in Fig. 2(a). At the start of the experiments, point A, state of charge (SOC) of the $LiFePO_4$ cathode was not known unambiguously. Therefore, after Li-foil cell was assembled, $LiFePO_4$ cathode was first charged in constant current – constant voltage (CC-CV) mode at C/20 rate to ensure 100% SOC, point B. The AFM images were collected continuously from point A to point D as shown in Fig. 2(a). The height, deflection and 3D AFM images at points C and D are given in Fig. 2(b). After point D, we were not able to collect AFM images due to tip degradation and contamination. We have analyzed the $LiFePO_4$ particles in areas 1 and 2 (Fig. 2(b)) for surface area change by comparing the images at the beginning of discharge (i.e., point C) and after 6 h of discharge (i.e., point D). In total four particles were analyzed as shown in Fig. 3(a). The reference feature shown in Fig. 2(b) by a dashed circle was utilized to identify the same particles in the images that were collected at different times (i.e., points C and D). We did not observe dramatic changes in the surface morphology after partial discharge. At point D, $LiFePO_4$ cathode is only discharged to a SOC of 70% which corresponds to 2% change in the volume of $LiFePO_4$ particles which indicates that particle surface area increase should be less than $\leq$ 2%. Out of four particles, particles 1 and 2 showed surface area increase around 2%; however, particles 3 and 4 showed 7.4% and 14.3% increase in surface area, respectively (Fig. 3(b)). Motif analysis of four different particles revealed that surface area increase in $LiFePO_4$ particles is not uniform which may be associated with the inhomogeneous current density and/or carbon black distribution in the cathode. We were not able to analyze sufficient number of particles to draw statistically significant conclusions on surface area change of $LiFePO_4$ particles due to difficulties in motif analysis by segmentation. Improved post processing techniques are required to analyze more particles in an automated fashion.
Industry Collaboration	• None at the moment
US-China Collaboration Activities	• In the recently conducted teleconference regarding the development of a battery database (centered at the University of Michigan) accessible by all CERC members, OSU presented its data structure for available battery data to both US and several Chinese partners of the project.

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)

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).

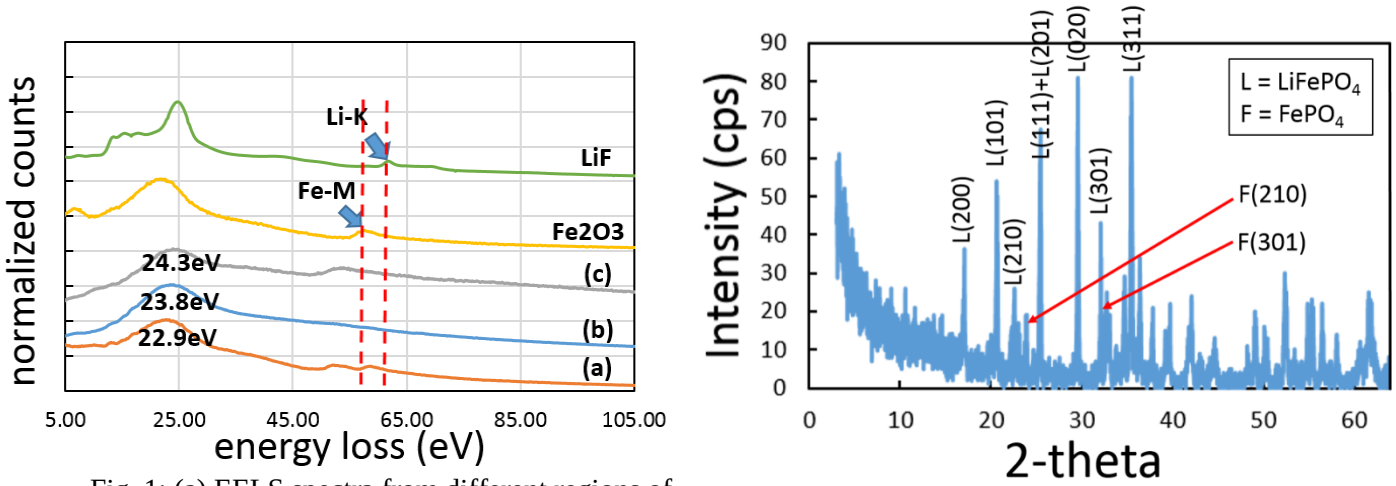


Fig. 1: (a) EELS spectra from different regions of a nanoparticle (b) XRD spectrum of a standard nanoparticle showing $LiFePO_4$ and $FePO_4$ peaks

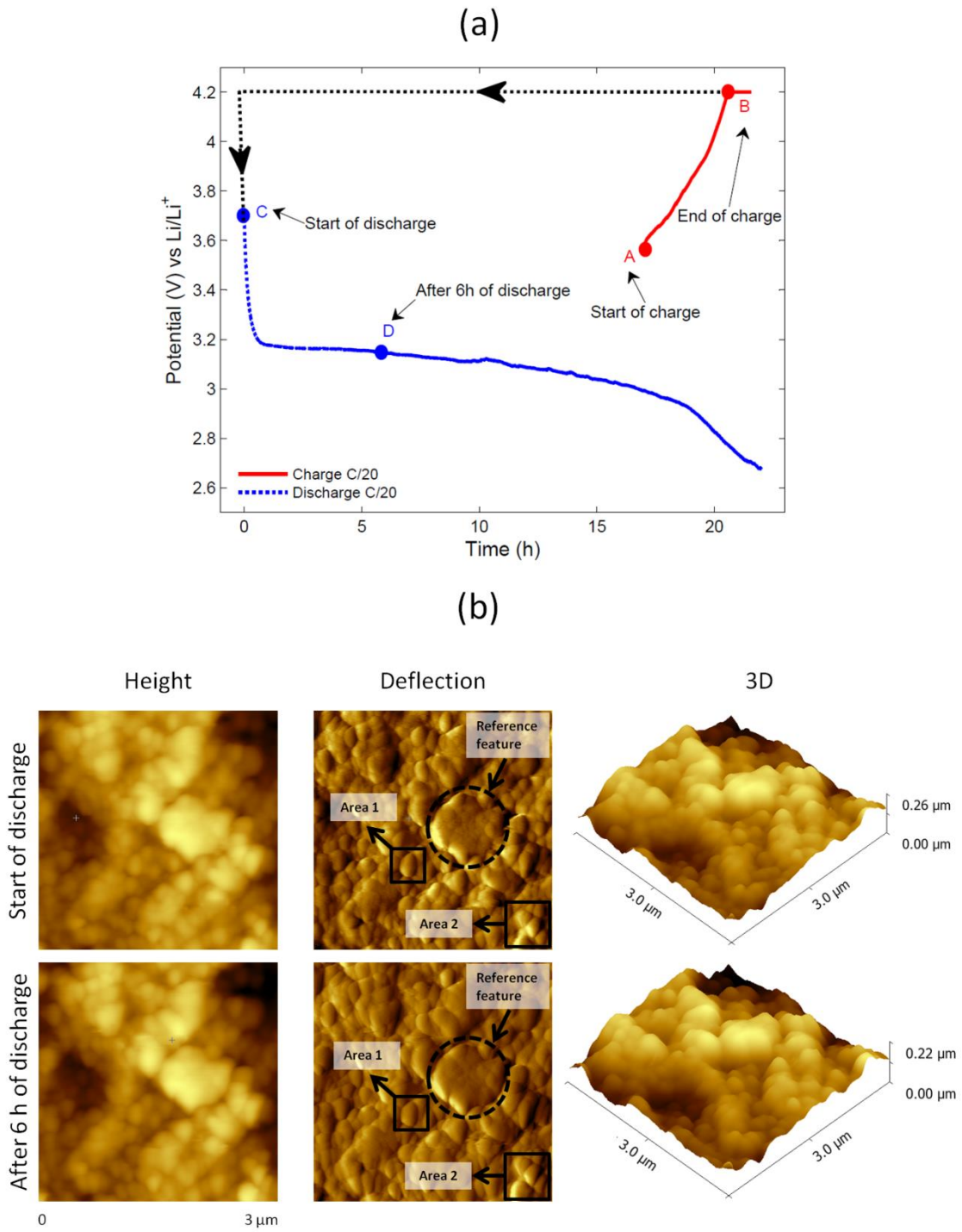


Fig. 2 (a) In situ $LiFePO_4$ half cell cycling data using Li-foil cell. (b) AFM images at the start and after 6 h of discharge. Reference feature was utilized to compare the particles at the beginning of the discharge and after 6 h of discharge. The particles in areas 1 and 2 were analyzed for surface area change during discharge as given in Fig. 3.

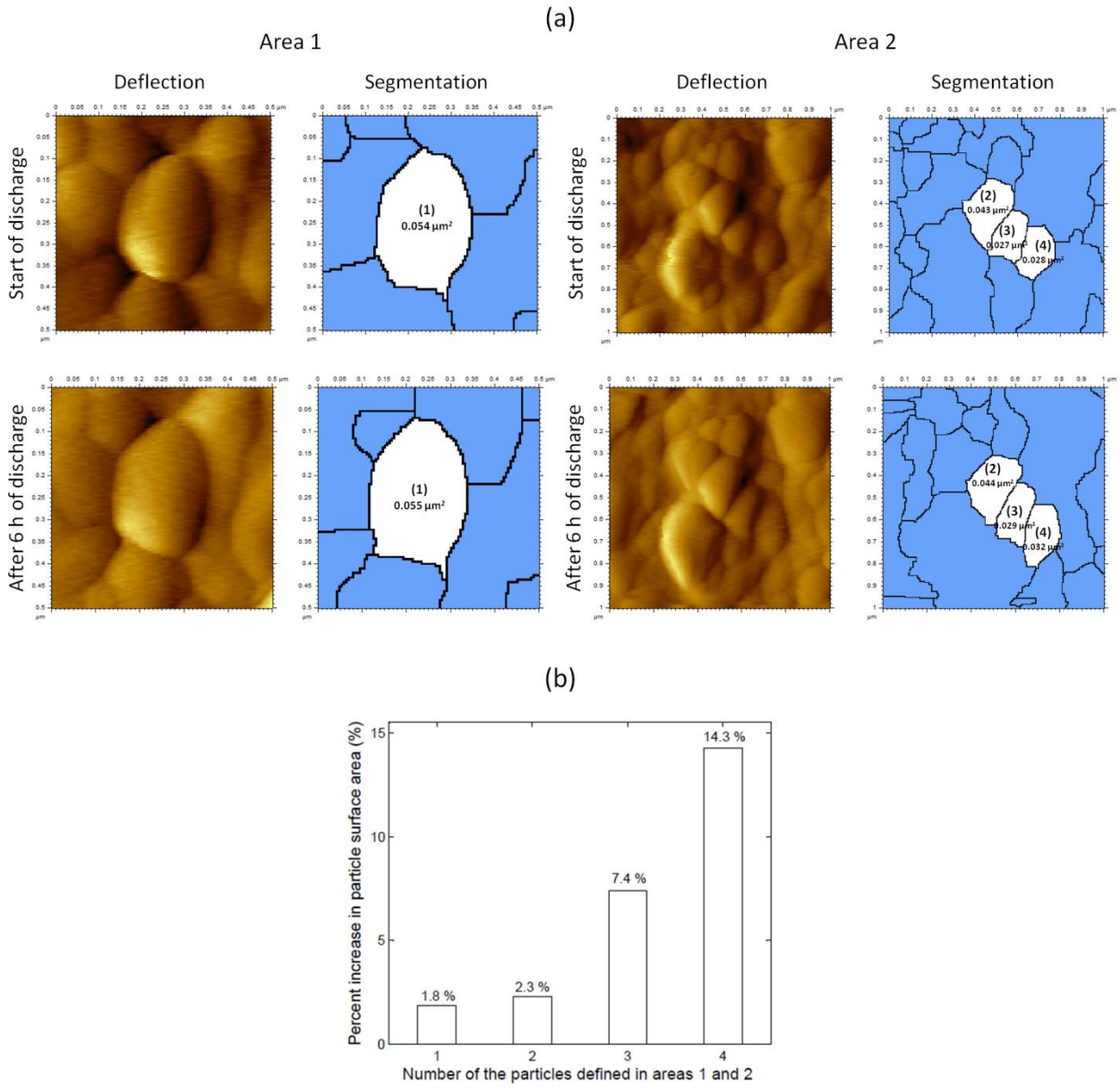


Fig.3 (a) Deflection and segmented images of areas 1 and 2 given in Fig. 3(b). Four $LiFePO_4$ particles were analyzed for surface area change, (b) percent increase in particle surface area after 6 h of discharge at C/20 rate.

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 (Cooperative US)**
Personnel	PIs: Marcello Canova (OSU), Raymond Cao (OSU), Anne Co (OSU) GRA: Jinghui Wang (OSU), Danny Liu (OSU)
Objective	• To establish a direct method to measure the lithium intercalation in the anode and cathode of commercial lithium-ion batteries; • To establish a technique to conduct in-situ measurement of the lithium concentration distribution in the anode and cathode of lithium-ion cells during cell utilization (discharging – charging); • To identify the effect of aging and shape factors on the lithium intercalation in anode and cathode through direct in-situ measurements. • To improve the accuracy of performance and aging models through better understanding of the relation between degree of lithiation and state of charge, diffusion kinetics and concentration in liquid and solid phase in the cell. • No changes in objectives or approach.
Progress Report	In this quarter we fabricated a sealed electrochemical cell (Fig.1 (A)) at OSU, and performed in-situ study using the NDP facility (Fig.1(B)) at NIST, the lithiation/delithation of a thin Sn foil (ca. 12.5 µm) were studied (Fig.1(C)). NDP spectra collected during charge/discharge cycles were recorded every 5 min during a potentiostatic hold at +0.4 V vs. Li/Li+ (lithiation) over a period of 12 hrs amounting to ca. 200 mAhr/g. The real-time evolution of the Li distribution at 60 min intervals is shown in Fig. 2. Prior to lithiation (Fig.2 black dashed line), Li signal in the electrolyte region (-5 to 0µm) of 6.2×10^{20} atom/cm^3 corresponds to the concentration of Li in 1M LiBF4. Upon lithiation, it is evident that an enrichment of Li at the near surface region (up to 2µm) of Sn is prevalent (0 to 260 min) followed by the diffusion of Li into the bulk. The surface concentration of Li reaches a steady state at 1.9×1022 atoms/cm3 by 680 min (equivalent to ca. 200 mAhr/g). The experiment conducted also elucidated an interesting phenomenon occurring in the electrolyte region. Fig. 2 shows an increase in the concentration of the electrolyte upon charge at relatively uniform increments with time. This increase can be attributed to increased concentration of Li salt due to solvent consumption during the formation of the SEI or due to a decrease in volume from the expansion of the electrodes. Another possible explanation is the preferential migration of ^{6}Li towards the Sn during lithiation induced enrichment of ^{6}Li. We exhibited that the kinetics of Li reactions, intercalation and transport by in-situ NDP, providing information that is indispensable in the advancement of materials for energy storage.
Industry Collaboration	• None at the moment. Collaborations with Industry and National Labs will be sought in 2014 to provide samples of electrodes to characterize with this technique.
US-China Collaboration Activities	• None at the moment
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," submitted to *Advanced materials*

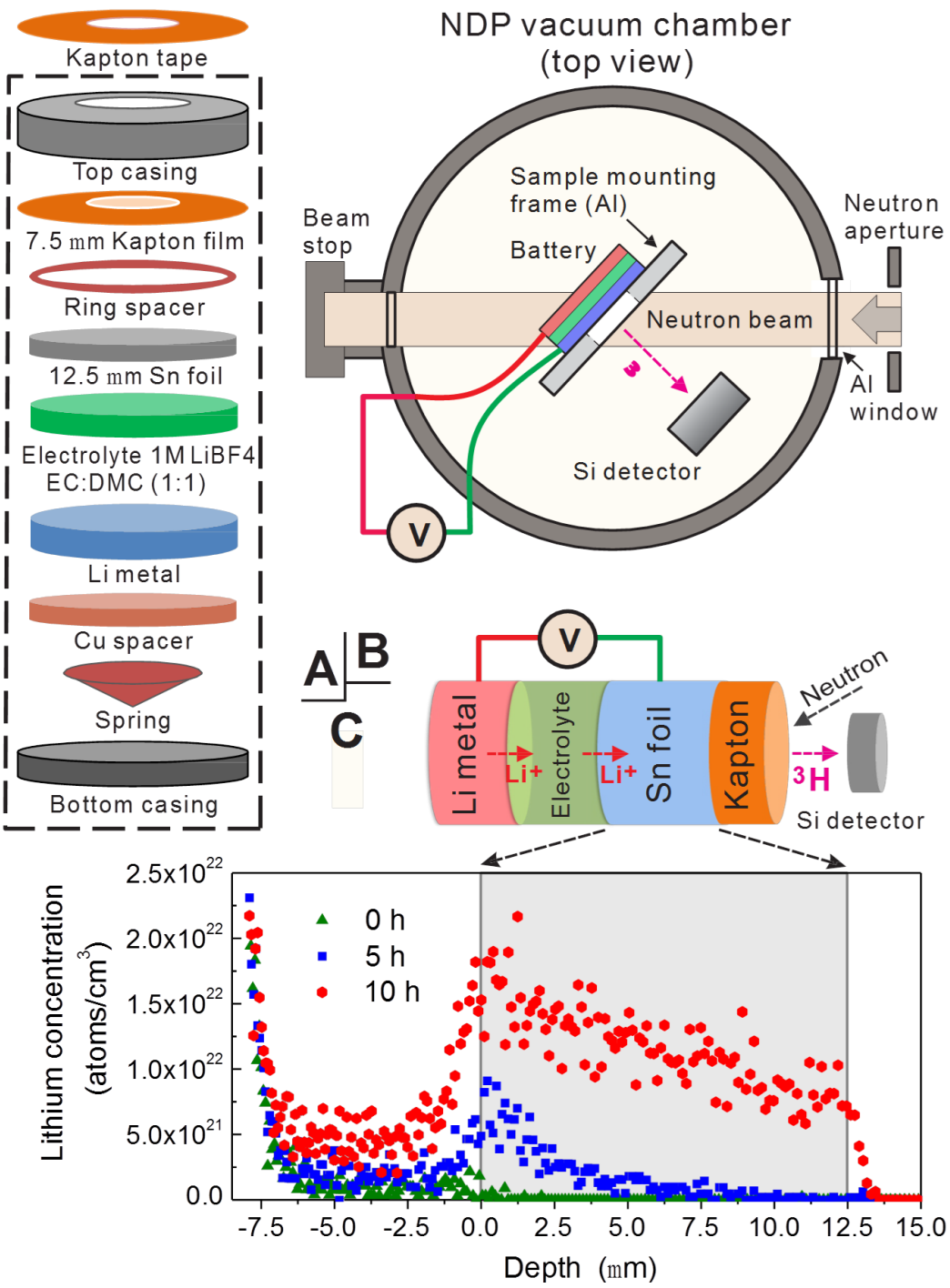


Fig. 1. (A) A schematic representation of the battery components; (B) illustration of the NDP set-up; and (C) a snap shot of the in-situ NDP spectra showing Li transport during charging/discharging a battery.

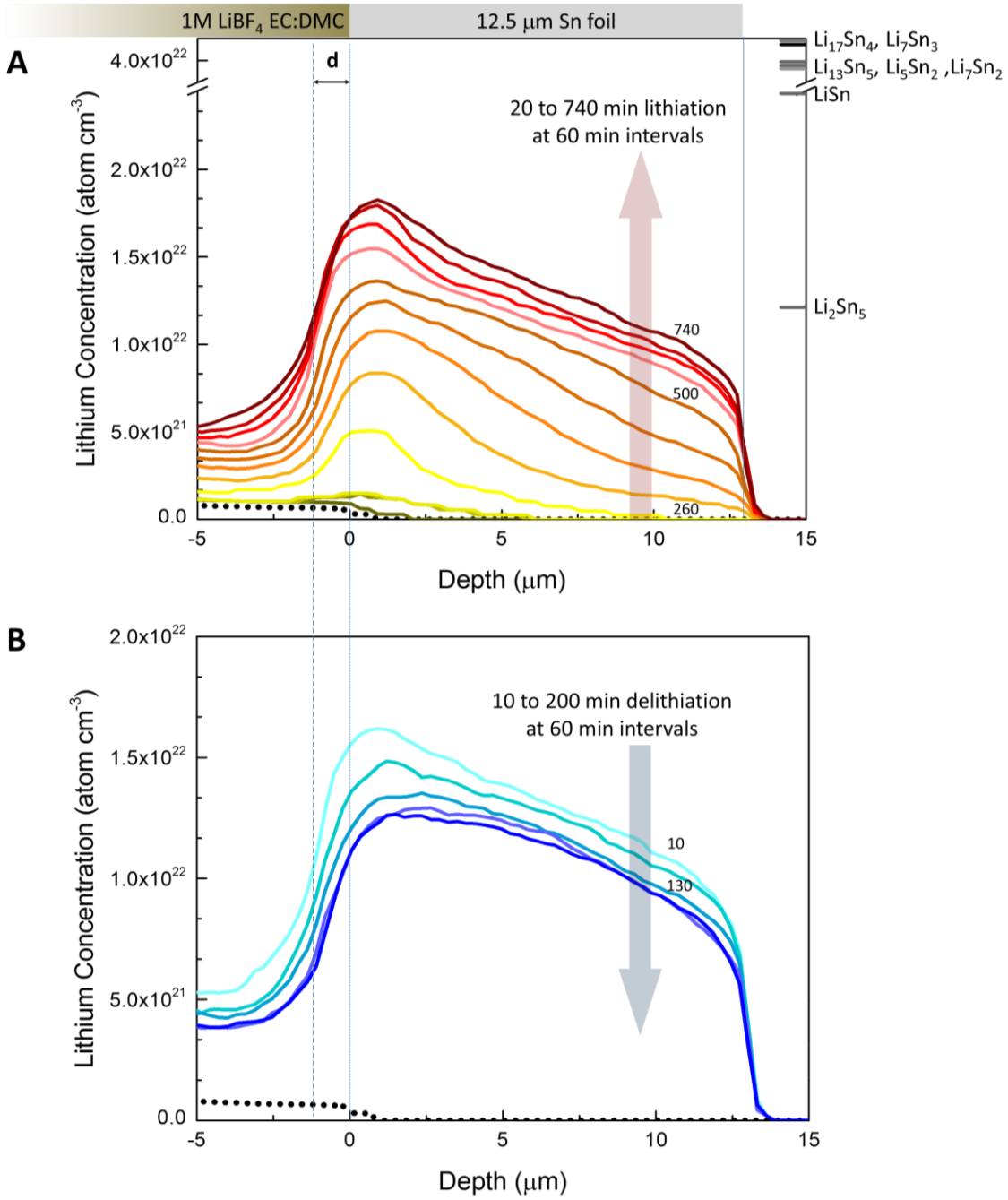
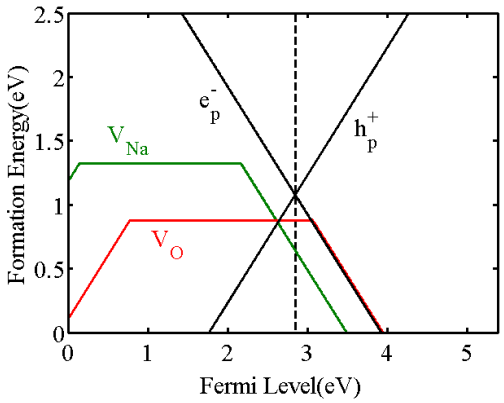


Fig. 2. Lithium concentration profiles within a 12.5 μm Sn foil as a function of time. (dashed) before electrochemical lithiation, (A) Lithiation spectra plotted every 60 min interval from 20 min to 740 min at 0.4 V vs. Li/Li^+(reaching approx. 200 mAhr/g); (B) Delithiation spectra plotted every 60 min interval from 10 min to 200 min delithiation at 1.0 V vs. Li/Li^+.

Thrust	TA 1: Advanced Batteries and Energy Conversion
Title	**Project 1.3: Li-ion Battery Aging and Internal Degradation Mechanisms (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	Li–O_2 (or Li-air) batteries have high theoretical specific energy which makes it a promising candidate for energy storage in electric vehicles (EVs). One of the main issues hindering the development of Li-O_2 batteries is decomposition of the organic electrolyte [1] which has been further associated with undesirable phenomena such as capacity fade, high charging overpotentials, and limited cycle life. Thus, a deeper understanding of these reactions is a crucial step in developing practical Li-O_2 batteries. To accomplish this, we are using first principles DFT calculations to study the initial decomposition reactions of the electrolyte solvent DME on peroxide-like and superoxide-like surfaces [2] of Li_2O_2, the primary discharge product in Li-O_2 batteries [1]. We find that DME adsorbs more exothermally on peroxide-like than on superoxide-like surfaces. Consistent with previous cluster calculations [3], the degradation reaction proceeds exothermically via hydrogen abstraction (H-abstraction) wherein a hydrogen detaches from either the CH_3 or CH_2 group of DME and bonds to surface O_2 dimers. On the peroxide-like surface, the H-abstraction results in dissociation of O_2 dimers, forming a surface hydroxyl (-OH) and a reactive oxide (O^{2-}) that participates in nucleophilic attack on the H-abstracted carbon of the DME. In contrast, H-abstraction on the superoxide-like surface leads to a stable (i.e., less reactive) O_2H surface species. The H-abstraction reaction is significantly more exothermic on peroxide-like than on superoxide-like surface. However, we find that the activation energy calculations indicate that DME is more susceptible to decompose on superoxide-like than on peroxide-like surfaces. In near future, we are planning to use the metadynamics technique to further study decomposition of DME on Li_2O_2 surfaces. [1] McCloskey, B. D.; Valery, A.; Luntz, A. C.; Gowda, S. R.; Wallraff, G. M.;Garcia, J. M.; Mori, T.; Krupp, L. E. Combining Accurate O_2 and Li_2O_2 Assays to Separate Discharge and Charge Stability Limitations in Nonaqueous Li–O_2 Batteries. *J. Phys. Chem. Lett.*, **4**, 2989–2993 (2013). [2] 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.* **2012**, *134*, 1093–1103. [3] Assary, R. S.; Lau, K. C.; Sun, Y.; Curtiss, L. A. Interactions of Dimethoxy Ethane with Li2O2 Clusters and Likely Decomposition Mechanisms for Li–O2 Batteries. *J. Phys. Chem. C*, ***117*** (16), 8041–8049 (2013).
Industry Collaboration	• In near future, we will be starting collaborating with U.S. industrial partner on studying the electrolyte interaction with high voltage spinel cathodes.

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	• **Publication:** Invited article in Journal of The Electrochemical Society's Focus Issue on Mathematical Modeling of Electrochemical Systems at Multiple Scales: Crystal Surface and State of Charge Dependencies of Electrolyte Decomposition on $LiMn_2O_4$ Cathode. Kumar, N.; Leung, K.; and Siegel, D. J. J. Electrochem. Soc. 2014 161(8): E3059-E3065; DOI:10.1149/2.009408jes • **Abstract Submitted:** "DME decomposition on Li_2O_2 surfaces: Role of peroxide and superoxide terminations" for oral presentation at 248th ACS National Meeting (San Francisco, CA) in the Modeling and Simulations of Electrochemical Interfaces and Materials for Energy Storage (COMP division) symposium. • **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 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.
Progress Report	We are continuing our modeling of the properties of discharge phases in Na-O_2 batteries. In these system both Na_2O_2 and NaO_2 are found to be reversible in experiments, however systems that discharge to NaO_2 (sodium superoxide) exhibit much lower overpotentials upon charging. As a step towards understanding these differences we are examining charge transport within the NaO_2 and Na_2O_2 phases. Our previous work demonstrated that both compounds have large bandgaps, suggesting that they have poor band conduction. An alternative conduction mechanism would involve migration of point defects or hopping of localized holes or electrons (polarons). We are currently exploring these transport mechanisms by calculating the conductivity arising from intrinsic defects in Na_2O_2 and NaO_2. These calculations will allow us to test our hypothesis that low charging overpotentials in NaO_2 arise from more facile transport compared to Na_2O_2. Figure 1 shows defect formation energies as a function of the Fermi energy (relative to the valence band maximum) in NaO_2. A hybrid functional (HSEα) was used with an α value tuned to match the bandgap calculated by quasi particle GW methods. Polarons and vacancies with different charge states were considered. Our calculations show that hole polarons and negative sodium vacancies are the dominant charge carriers.  **Figure 1.** Formation energies of various point defects in NaO_2(pyrite). Positive defects have an upward slope while negative defects have a downward slope. The vertical dashed line represents the position of the Fermi level calculated from charge neutrality.
Industry Collaboration	• Monthly teleconferences were held amongst U.S. researchers and industrial partners.
US-China Collaboration Activities	
Issues of Concern	None.
Notable Recent Achievements	Invited presentation: • (D. Siegel) American Ceramic Society -- Electronic Materials & Applications Conference, January 22-24, 2014, Orlando, FL.

Thrust	TA 1: Advanced Batteries and Energy Conversion
Title	**Project 2.2: Fundamental Understanding of Li-Air Reaction Mechanisms (Joint)**
Personnel	PIs: Yang Shao-Horn and Gerbrand Ceder (MIT) Graduate students: David Kwabi (50%) and ShinYoung Kang (50%) (MIT)

Objective	Stemming from Li−O_2 batteries, which have high theoretical energy, but the industry level adoption of which is limited due to such as low round-trip efficiency and poor cycle life, we expanded our interest to general metal−O_2 batteries. While we keep investigating the underlying reaction mechanisms in Li−O_2 cells, we also study the fundamental thermodynamics in Na−O_2 cells.
	• In order to address the question why some Na−O_2 cells form Na_2O_2 as a discharge product, while others form NaO_2 based on the phase diagram, we investigate
	  ○ the thermodynamic stability of various bulk sodium oxides (e.g. Na_2O, Na_2O_2, NaO_2 and NaO_3) using first-principles calculations
	  ○ a phase diagram of sodium oxides as a function of particle size, temperature and O_2 partial pressure constructed based on the calculated bulk formation energies and surface energies of sodium oxides
	• In Li−O_2 batteries, study the thermodynamics and kinetics of the decomposition of discharge products and characterize the involved species using x-ray diffraction (XRD) and spectroscopies.

Progress Report	• We found even though Na_2O_2 is a stable phase in bulk at the standard state (300 K, P_{O2} = 1 atm), at nano-scale low surface energies stabilize NaO_2 nano-particles up to 6 nm at the standard state. • Such NaO_2 nano-particles are rather facile to nucleate due to their lower nucleation energy barrier and smaller critical nucleus size compared to Na_2O_2 particles. • In addition, considering distinct crystal structures between Na_2O_2 and NaO_2, NaO_2 nano-particles may be able to grow to micro-size as observed in experiments. • We have investigated the decomposition of products of the Li−O_2 discharge reaction by dimethyl sulfoxide, which is a popular electrolyte solvent for Li−O_2 batteries. The presence of superoxide-related species in accelerating this decomposition was established via XRD, as well as Raman and FTIR spectroscopy.
Industry Collaboration	None
US-China Collaboration Activities	None
Issues of Concern	None
Notable Recent Achievements	Kang, S.; Mo, Y.; Ong, S. P.; Ceder, G. (2014). "Nanoscale Stabilization of Sodium Oxides: Implications for Na-O2 Batteries." *Nano Letters* **14**(2): 1016-1020.

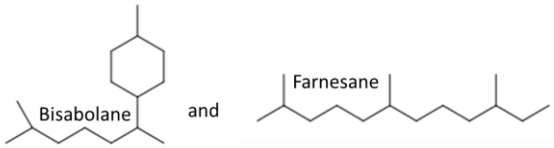
Thrust Area 2: Clean Combustion and Energy Conversion

Thrust	Thrust 2: Advanced Biofuels, Clean Combustion and Auxiliary Power Unit (APU)
Title	**Project 1: Biofuel Chemistry & Physics (Joint)**
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: ortho-xylene, meta- xylene, para- xylene • Determination of the effect of temperature on competing chain-propagation and chain-termination channels

Progress Report	• Seven molecules studied to-date: (1) 2,5-dimethylhexane; (2) o-/m-/p-cymene; (3) o-/m-/p-xylene
	• Continued the investigation of key features related to a low-temperature ignition phenomena (the *ortho*- effect) characteristic of substituted aromatics which are relevant to diesel and gasoline applications (see list below). The effects of resonance stabilization of initial radicals or of key intermediates can have significant impact on substituted aromatic oxidation.
	  ○ Temperature-dependence of the ortho- effect in xylenes is more dramatic than in cymenes because only resonance-stabilized initial radicals are produced
	  ○ The primary low-temperature fuel consumption pathways were quantified using branching fraction measurements performed at the Advanced Light Source of Lawrence Berkeley National Laboratory
	• Paper on results from cymene experiments and modeling in revision at *Proceedings of the Combustion Institute* (ISSN: 1540-7489)
	• Completed: calculations of isomerization kinetics for 2,5-dimethylhexyl radicals
	• Completed: New photoionization mass spectrometry measurements of aromatic fuels (cymenes, xylenes)

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 • Post-doctoral fellows trained (Rotavera, Sandia; Ali, U. Michigan)
Issues of Concern	None
Notable Recent Achievements	• Report on cymene oxidation accepted for presentation to the 35th International Symposium on Combustion (to be held in August 2014)

Thrust	Advanced Biofuels, Clean Combustion and Auxiliary Power Unit (APU)
Title	**Project 1.2: Chemical and Physical Models for Novel Biofuels (Cooperative US)**
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
Progress Report	The escalating costs of fossil fuels, along with the eventual need to replace fossil fuels entirely, has led researchers to investigate alternative means of producing energy. Specifically, the need to replace liquid fuels for mobile internal combustion engines has motivated researchers to evaluate bio-derived fuels as an alternative to diesel fuels.[1] Peralta-Yahya et al.[2] have synthesized novel bio-derived fuel molecules such as bisabolane (e.g. 1-methyl-4(6-methyl-2-heptanyl) cyclohexane) and farnesane (e.g., 3,7,11-trimethyl-dodecane) whose structures are shown in Fig. 1. 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 the low temperature oxidation of 2,5-dimethylhexane (a bisabolane fragment); in this quarter we have continued our investigation of 2,5-dimethylhexane, specifically focusing on the high temperature decomposition of the fragment. In this quarter we compiled all the reactions and their corresponding reaction rates into a sub-mechanism that describes the decomposition of the fuel and subsequent dissociation of the intermediates. This sub-mechanism was then incorporated into an existing "base mechanism" that describes the evolution of the system of smaller species created by our sub-mechanism. This new model that describes the evolution of 2,5-dimethylhexane was used to simulate the behavior of the fuel in several situations, including shock tubes, rapid compression machines, and closed homogeneous reactors. We used these ignition delay experiments to validate our model. When comparing simulations with experiments, we noticed discrepancies that we could ameliorate by refining the model. We performed sensitivity analyses and rates of production analyses in order to tease out the reactions that influence the ignition delay most significantly. As it turns out, the reactions that most influenced ignition delay were in the "base mechanism" and those rates were estimated, not calculated. Therefore, we could justify altering these rates; we then modified the rates of these few reactions according to literature. Subsequent simulations with the updated mechanism demonstrated an improvement in the predictive capabilities of our model. We are currently working on further refinement – trying to reduce the discrepancies between experiment and simulation. The difficulty in developing a "good" deterministic model for fuel oxidation is fitting it to multiple experiments that are conducted in a wide range of initial temperatures and pressures and equivalence ratios. However, though more difficult and time-consuming, the method of validating

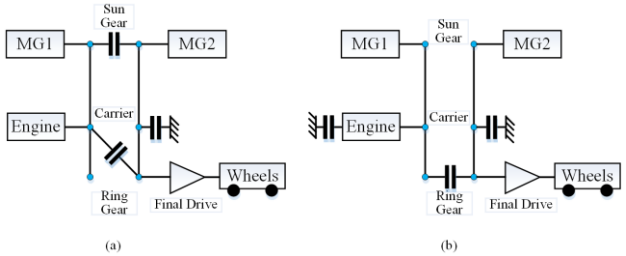
	our model with many different experiments ensures that our model is very robust. We expect in the next quarter to have results demonstrating the ability of our model to predict the oxidation of 2,5-dimethylhexane in a wide range of pressures and temperatures. **Figure 1.** Structures of novel biofuel molecules.  **References** [1] Lai, J.Y.W.; Lin, K.C.; Violi, A. *Progress in Energy and Combustion Science* **2011**, *37*, 1-14. [2] Peralta-Yahya P. P.; Ouellet M., Chan, R. Mukhopadhyay, A. Keasling, J.D. Lee, T. S. *Nature Communications* **2011**, 2, 483.
Issues of Concern	Because we were unable to acquire farnesane, we attempted to chemically hydrogenate farnasene. This process proved untenable for various reasons, mostly that is is too time-consuming to generate a quantity large enough for engine experiments which requires on the order of a couple gallons of fuel. Despite this setback, we decided to continue to pursue the development of bisabolane and farnesane mechanisms. It would set back the research too much if we started over with a fuel that was immediately obtainable.
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	N/A
Notable Recent Achievements	N/A

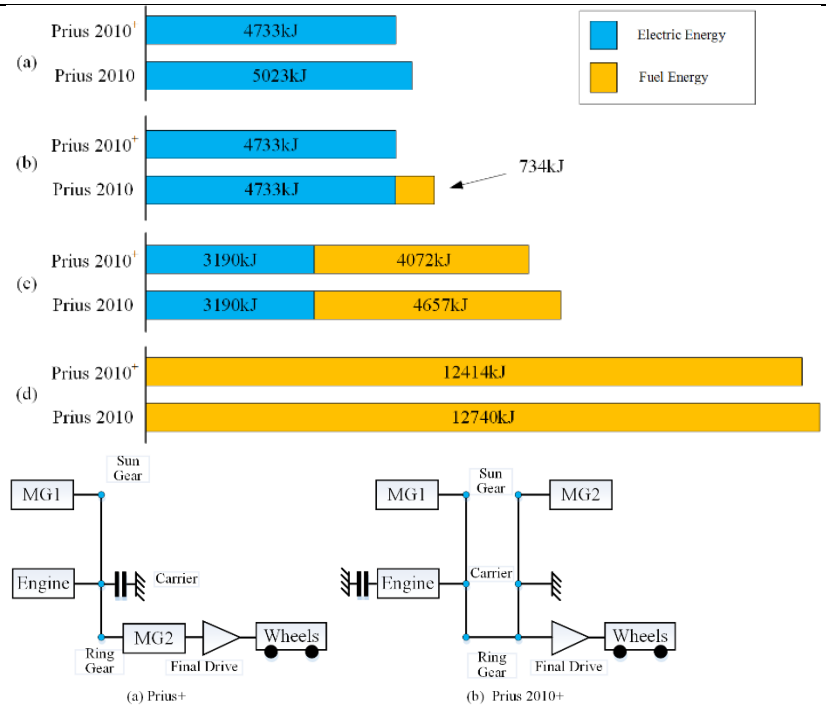
Thrust	TA 2: Advanced Biofules and Clean Combustion
Title	**Project 2: Integrated Powertrain and Aftertreatment System Control for Clean Vehicles (Joint)**
Personnel	PI: Junmin Wang (OSU), Jim Parks (ORNL), Fuyuan Yang (THU), Graduate student: Junfeng Zhao (OSU)
Objective	The objective of this project 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	• Developed and experimentally validated methods for simultaneous estimations of fuel blend level and intake manifold oxygen concentration. • 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	The following 4 peer-reviewed papers have been published or accepted for publication, and several other manuscripts are under review. 1. Junfeng Zhao and Junmin Wang, "Adaptive Observer for Joint Estimation of Oxygen Fractions and Blend Level in Biodiesel Fueled Engines," IEEE Transactions on Control Systems Technology (in press), 2014. 2. Junfeng Zhao and Junmin Wang, "On-Board Fuel Property Identification Method Based on High-Pressure Common Rail Pressure Signal," ASME Transactions Journal of Dynamic Systems, Measurement, and Control, Vol. 136, No. 3, 031010 (9 pages), 2014. 3. Pingen Chen and Junmin Wang, "Control-Oriented Model for Integrated Diesel Engine and Aftertreatment Systems Thermal Management," *Control Engineering Practice*, Vol. 22, pp. 81 – 93, 2014. 4. Junfeng Zhao and Junmin Wang, "Engine Mass Airflow Sensor Fault Detection via an Adaptive Oxygen Fraction Observer," Proceedings of the 2014 American Control Conference (Invited Paper) (accepted), 2014.

Thrust	TA 2: Project 4
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. Yb-filled and Sn-doped $CoSb_3$ samples fabricated and undergoing transport measurements. 2. A new joint paper with WHUT published on the relevance of single parabolic band model to $Mg_2Si_{1-x}Sn_x$ solid solutions. 3.
Industry Collaboration	None, but discussions with potential industrial partners in progress.
US-China Collaboration Activities	Prof. Uher visited the Wuhan University of Technology during March 16-23, 2014.
Issues of Concern	None
Notable Recent Achievements	• S. Hui, M. Nielson, D. Medlin, J. Salvador, J.P. Heremans, K.P. Pipe, and C. Uher, "Influence of Doping on the Thermoelectric Transport Properties in $CoSb_3$-based Skutterudites", accepted for publication *in Journal of Applied Physics*. • 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*. DOI:10.1039/C4Cp00641K (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	• Develop computationally efficient finite element tools for electric machine design
Progress Report	We have submitted a manuscript on the existing harmonic balance/domain decomposition algorithm for synchronous machines to ECCE 2014. We have also prepared a journal paper based on our previous work on the application of diagonally-implicit Runge-Kutta (DIRK) integration methods to the shooting-Newton algorithm. We have also extended the application of the DIRK methods to another time-domain steady-state called the time-periodic finite element method. Until now, these methods have never undergone a rigorous comparison. We have shown that they achieve similar performance for a typical use case by simulating a surface-mount permanent magnet machine, with the shooting-Newton method being somewhat faster in the example under study. The time-periodic finite-element method has been applied to induction machines using a polyphase time-periodic condition to improve simulation speed. This condition increases the number of slip frequencies which can resonably be analyzed. We believe the same technique can be applied to the shooting-Newton method. Because induction machines have larger time-constants than SMPM machines, and the shooting-Newton method performs better than the time-periodic finite-element method when the time constants are large, we anticipate significant improvements for serial implementations. We are also in the planning stages of validating our code against results collected from hardware.
Industry Collaboration	• The developed finite element codes are being used by a postdoctoral student, Zifu Wang, on a separately-sponsored project funded by DENSO, a CERC member. • The Ph.D. student supported on this project, Jason Pries, will be visiting Oak Ridge National Labs for 6 months between mid-April and mid-October.
US-China Collaboration Activities	• We are hosting a Tsinghua student, Ziyou Song, who will be working in our research laboratory for one year.
Issues of Concern	• None
Notable Recent Achievements	• Development of computationally efficient steady-state FEA solver for induction machines.

Thrust	TA3: Vehicle Electrification
Title	**Project 3.1 Rapid system integration through modular configuration, sizing and control (Joint)**
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), Prof. Geng Yang (THU), Prof. Zhichao Hou (THU), Prof. Yu Zhu (SJTU) Graduate Students: Xiaowu Zhang (UM), Andrea Cordoba (UM), 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 previous quarters, we reported our effort in combining PEARS – a fast optimization method, together with automated modeling and mode identification approach to find the optimal clutch location for configuration #83. We limit the clutch number to 3, which gives us C_{16}^{3} different possible locations. The optimization results show that for fuel economy based on 55/45 weighting of city and highway cycles, 50 different designs achieve better fuel economy in HEV (charge sustaining operation) compared with the Toyota Prius configuration. Two of the example designs are shown below:  • Over the last quarter, we extended the systematic design procedure from using two planetary gears to designs with multiple planetary gear and clutches. All possible configurations and clutch locations can now be calculated systematically, including those using Ravignaux planetary gears. • A more systematic coding for multiple planetary gear design has been programmed with significant efficiency improvement. • After consulting with researchers in Ford research labs, we designed an in-depth energy flow analysis to better understand the source of improvement in energy consumption due to multiple-mode operations. Prius 2010 is the design is MY 2010 Prius and the "Prius 2010+" design one of the 50 designs identified by our systematic design process that achieves superior fuel economy. The "Prius 2010+" design is very similar to the Prius 2010 design but with an extra clutch. Incidentally, the location where a clutch was added is the same as the "Prius+" design proposed earlier by this research.

	• 
Industry Collaboration	• The comprehensive 1PG design and analysis results have been presented in our TA project review meeting to all CERC industrial members. We also held a separate meeting to seek comments from Ford HEV expert Ming Kuang. • We are collaborating with Ford to start Power-split Hybrid F150 project. Three meetings were held during the past quarter.
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 arrived in February 2014 in Ann Arbor for a one-year exchange. Both of them are hosted by Prof. Huei Peng.
Issues of Concern	N/A
Notable Recent Achievements	• The paper published by 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" in 2013 American Control Conference was selected to receive the Best Paper Award by ASME Automotive and Transportation Systems Technical Committee.

Thrust	TA 3: Vehicle Electrification
Title	**Project 3.2: Intelligent Fault Diagnosis and Prognosis (Joint)**
Personnel	PI: Prof. Giorgio Rizzoni (OSU) Co-PI: 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. In the initial phase, we have analyze the number of sensors and their placements for better health monitoring of AMT. We are now working on sequential residual generators for FDI of 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. Initial simulation results are encouraging and we are trying to validate FDI scheme for battery system experimentally. • We have also applied the FDI scheme based on structural analysis for PMSM drive system in an electric vehicle. We have conducted the detectability and isolability analysis for PMSM drive system given the possible sensor and fault locations. The next step will be focused on developing feasible residual generators to realize the isolability of various types of faults.
Industry Collaboration	• We are currently seeking partnerships with industrial collaborators to find vehicle applications of these methods beyond the OSU EcoCAR. One potential collaborator is JAC in Hefei, Anhui, China
US-China Collaboration Activities	• Prof. Rizzoni attended annual CERC Meeting in Beijing in April 2013. • 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. • 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	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*, submitted to 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*, submitted to DSCC 2014

	3. Qi Chen, Qadeer Ahmed and Giorgio Rizzoni, *Sensor Placement Analysis For Fault Detectability And Isolability Of An Automated Manual* submitted to DSCC 2014 4. Jiyu Zhang, Andrea Cordoba-Arenas, Giorgio Rizzoni, *Fault Diagnosis for PMSM Drive System in Electric Vehicle*. Submitted to DSCC 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 first 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. Inspired by our previous success on incremental capacity analysis (ICA) based lithium ion battery SOH monitoring with support vector regression (SVR), the team is looking into the possibility of efficient multi-cell battery system identification using support vector based model parametrization. Parametric battery model could be developed from single cell data and applied to other cells in the same pack. Comparing to applying SVR to every individual cell, the parametric model saves a significant amount of computational load, which is crucial for on-board battery SOH monitoring. The parametric structure of the model could also help us to better understand the aging mechanism of lithium ion batteries and the staging phenomenon during intercalation process. Our research activities in the first quarter of 2014 have been focused on (a) Analysis of the invariance of the support vectors for the parametrization of battery charging curves; (b) Using a mechanistic battery prognosis model to simulate battery aging process, and to correlate the simulation results with the mathematical analysis; (c) Establishing battery pack model and preparing for pack tests. For parts (a), the SVR based battery SOH monitoring problem is reformulated as a nonlinear multi-parametric linear programming (MLP) problem, in which the battery aging reflected in the measured voltage is treated as variations in the constraint vector. The variation is further approximated using quardratic function as shown in Fig. 1 and parametrized as, $y' = p_2 y_0^2 + p_1 y_0$ where y_0 is the voltage measurement of the reference cell, and y' is the voltage measurement of the cell being identified. The constant term is ignored in the quardratic function because it does not affect the optimality of the LP optimal basis. Following the general approaches for solving MLP problems, the corresponding feasible region for the parameters of the quardratic function to the initial optimal basis can be found using Monte Carlo simulation results (Fig. 2). That is, for any pair of p_1 and p_2, if the corresponding y' share the same set of optimal basis as y_0, (p_1, p_2) is considered feasible and plotted in the blue region in Fig. 2.

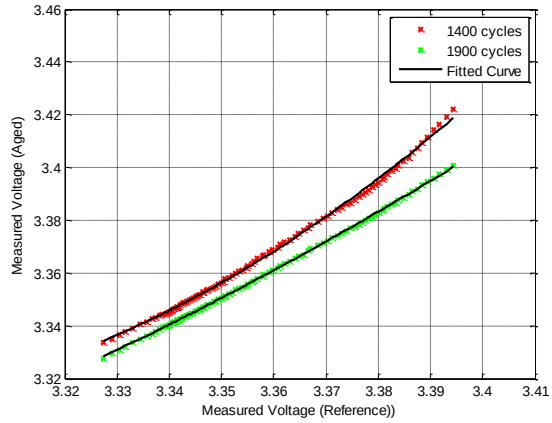


Figure 1: Approximation of measured voltage variation with quardratic function

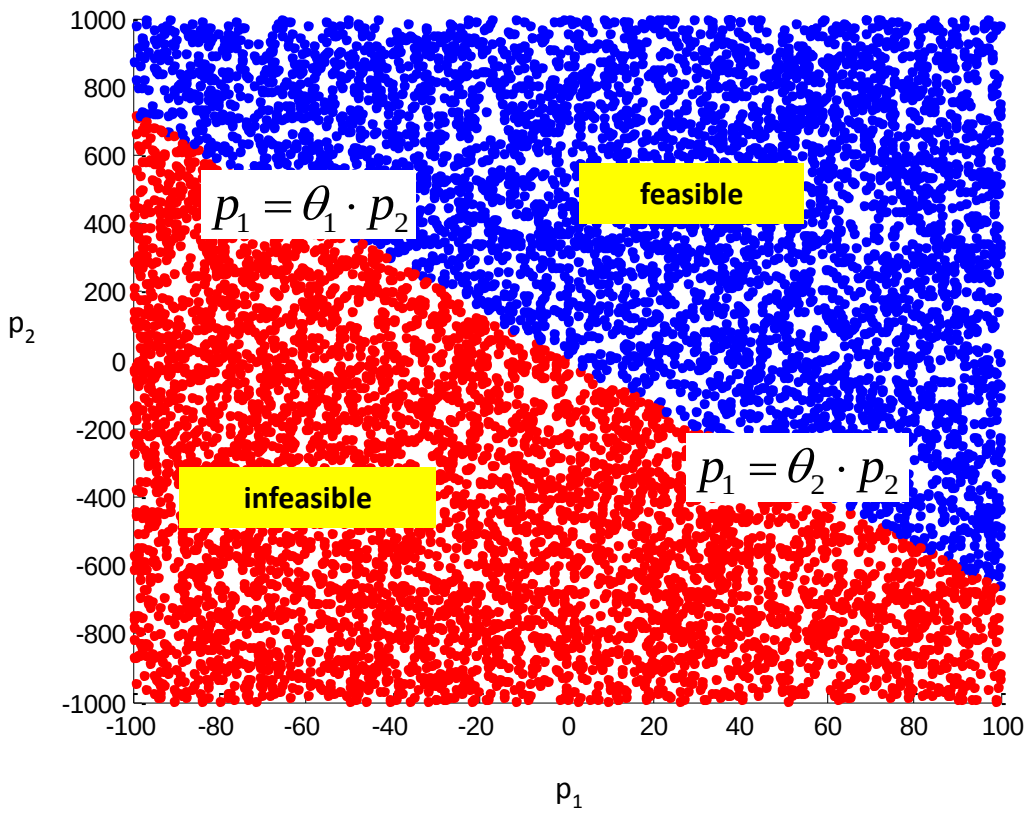


Figure 2: Feasible for function parameters corresponding to the initial optimal basis

From the results shown in Fig. 2, one can see that the feasible region is constrainted by linear relationships between p_1 and p_2. Since the ratio of p_1 over p_2 define the inflection point of the parabola, the linear relationships imply that the support vectors for the battery charging curve model would stay invariant as long as the variation in the voltage data satisfies a monotonic quardratic relationship. This result is consistent with our observations from the battery data.

For part (b), the variation pattern of the battery charging voltage is simulated using a mechanistic prognosis model which considers the loss of active material at positive and negative electrode as well as the loss of cycable lithium for battery capacity loss. The simulation results show that for battery chemistry such as the LiFePO4, the voltage variation does satisfy a quardratic and monotonic pattern and therefore the invariant

	properties of support vectors can be generalized and used as parametrization and adaptation tool for battery SOH monitoring. The battery pack model for part (c) is constructed to simulate more complex battery operating conditions due to the battery self-balancing in a parallel configuration. The prognosis model from part (b) that simulates the aging of battery OCV is also incorporated. The simulation show that SV based model parametrization and battery SOH monitoring could be extended from single cell to a multi-cell setting. Battery pack tests have also been designed for the verification of the simulation results. In the next quarter, the team will continue to focus on the development of adaptive battery management system. Efforts will be directed to battery pack testing. The developed battery SOH monitoring framework would be implenmented in multi-cell configuration. The aging mechanism associated with battery pack connection may also be studied.
Industry Collaboration	• Initial contact made with Delphi, who expressed interest as the industrial sponsor for increased collaboration and accelerated commercialization.
US-China Collaboration Activities	• A student from Tsinghua University started his one-year visiting and joint research program at the University of Michigan.
Issues of Concern	
Notable Recent Achievements	• A paper on OCV model for SOC and SOH estimation was accepted and published on the Journal of Power Sources

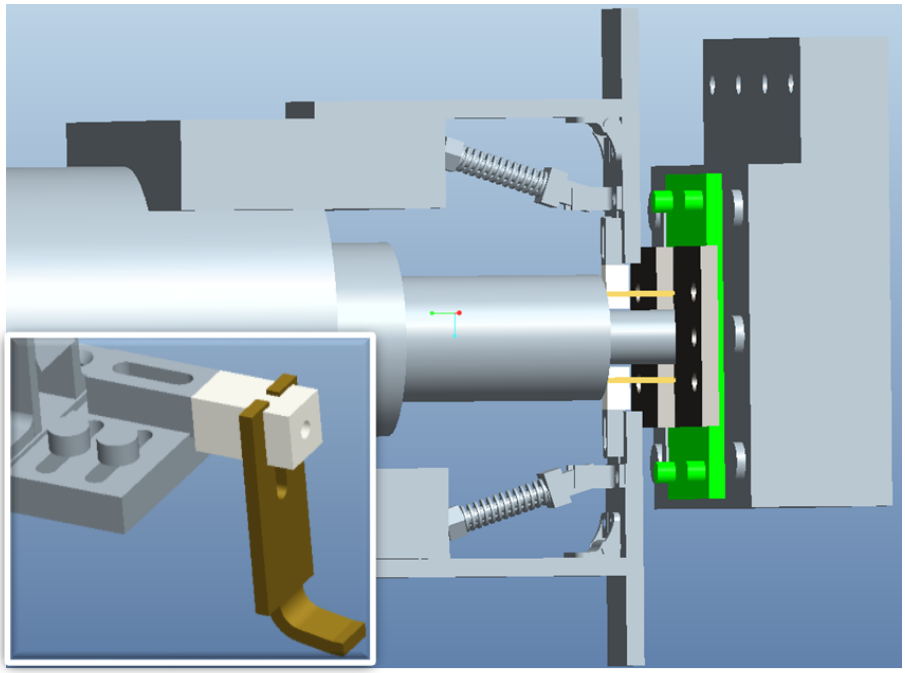
Thrust	TA 3: Vehicle Electrification
Title	**Project 4.2: Data-Based Techniques for Battery-Health Prediction (Cooperative US)**
Personnel	PIs: Jeffrey Stein, Dennis Bernstein (UM) Research Scientists: Tulga Ersal (UM) Graduate students: Xin Zhou (UM)
Objective	• Develop and demonstrate a novel, noninvasive approach to battery diagnostics. This approach, called Retrospective-cost-based Subsystem Identification (RCSI), uses data obtained from only noninvasive measurements to estimate health-relevant features of a battery that are otherwise hidden. • Using numerical computation, apply RCSI to models of Li-Ion batteries to estimate features of the battery-health subsystem. The research objective is to assess the accuracy of RCSI under realistic modeling errors and data limitations. • Using laboratory experiments validate the accuracy of the battery-health subsystem under laboratory conditions by comparing RCSI predictions to actual battery performance. • Demonstrate the ability of RCSI with noninvasive data to make accurate assessments and predictions of battery health.
Progress Report	• Switched to using the side reaction current density as the state of health indicator instead of the solid-electrolyte interphase film resistance. The choice of the side reaction current density enables the application of this algorithm in all electrochemical-based degradation mechanisms that is related to the side reaction. • Applied RCSI to the nonlinear battery model in simulation. Under the assumption that there is no noise or initialization error, RCSI was found effective for side

	reaction current density estimation during slow/fast constant current charge and discharge cycles and Urban Dynamometer Driving Schedule cycles. • Submitted a paper containing the results of the side reaction current density estimation to 2014 ASME Dynamic Systems and Control Conference.
Industry Collaboration	None.
US-China Collaboration Activities	None.
Issues of Concern	None.
Notable Recent Achievements	None.

Thrust Area 4: Advanced Lightweight Materials and Structures

Thrust	TA 4: Advanced Lightweight Materials and Structures
Title	**Project 2: Cost effective lightweight materials (Cooperative US)**
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 vehicles. The critical 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 approach when surface protection or surface conductivity is desired is to locate a carbon nanofibers (CNF) nanopaper on the surface of the glass fiber preform previous to resin impregnation.
Progress Report	In the past three months, a series experiments were carried out to investigate the effect of spraying nanoparticles on the surface of the preform or using a nanopaper on the surface of the preform on flexural properties. We have demonstrated that spraying about 5 weight percent of carbon nanotubes (CNT) will extend the elongation to break of the composite. We have also evaluated the effect on the elongation to break of the composite using CNF nanopaper. To make the nanopaper, both PANI and acid treatment were used to functionalize CNF nanoparticles. Previous experiments showed that CNF-PANI nanopaper has a higher tensile strength than CNF-Acid treated nanopaper since acid shortened the length of CNF. Our results show that CNF-PANI nanopaper on top (compression side) will help composites last longer than composites without nanopaper during 3-point bending test. Even at a strain of 10%, the sample won't fail. CNF-PANI nanopaper on the bottom (tension side) will still help composites last longer but the improvement is less. Composites sample breaks at a strain between 5%-6%, where without nanopaper fails at a strain of 3%. On the other hand, CNF-Acid treated nanopaper does not improve the elongation to break.
Industry Collaboration	• Nano Materials Innovation, a spinoff company from OSU, collaborates in the surface modification of nanoparticles.
US-China Collaboration Activities	• None.
Issues of Concern	• The flow through the nanopaper is difficult, this will slow down the composite fabrication process. It is critical to properly select gate locations, to minimize this issue.
Notable Recent Achievements	• Permeability Measurements and Flow Simulation for Polyaniline (PANI) Carbon Nano Fibers (CNF) Modified Nanopaper on Glass Fiber Preform, Submitted to Journal of Polymer Composites, under review • Permeability analysis of carbon nanofiber nanopapers, paper was accepted for presentation at the polymer processing 2014 annual technical conference (PPS30).

Thrust	4: Advanced Lightweight Materials and Structures
Title	**Project 3.2: Joining in Multi-Material Structures (Cooperative US)**
Personnel	Prof: Glenn S. Daehn (OSU) Graduate Student: Steven Hansen, (OSU)
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. • Next, effort will be put toward investigating longer continuous sheet-to-sheet solid-state welds using the vaporizing foil actuator technique, while continuing to work to understand and characterize the vaporizing foil launch process. This will allow application of this method to useful auto-body components.
Progress Report	• Experiments varying the flyer material and thickness in addition to the foil thickness and input energy are nearly complete, following the arrival of a replacement Rogowski current waveform transducer. Velocity (using photonic Doppler velocimetry), voltage, and current histories are recorded for all experiments. Analysis of the results is ongoing. • Continuous welds 3.5" long were demonstrated repeatedly between 0.74 mm thick AA6061T6 sheets. This is the longest weld able to be made using the current foil actuator setup; a different setup is in the works.
Industry Collaboration	• None
US-China Collaboration Activities	• No significant interactions this period.
Issues of Concern	
Notable Recent Achievements	**Published:** 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:** S.R. Hansen, A. Vivek, G.S. Daehn, "Vaporizing foil actuator: controlling the pressure pulse for impulse metalworking," Proceedings of the 2014 ASME Manufacturing Science and Engineering Conference.

Thrust	TA 4: Advanced Lightweight Materials and Structures
Title	**Project 3.3: Joining multi-material vehicle structures (Joint)**
Personnel	PI: Prof. Jun Ni (UM) Post Doc: Shuhuai Lan (UM) Graduate student: Xun Liu (UM)
Objective	Develop high-quality and economical joining processes between dissimilar lightweight materials.
Progress Report	A CNC machine has been adapted for electrically assisted friction stir welding process. The CAD design is shown in Fig.1. In order to guarantee close contact between electrodes and workpiece, two springs were mounted in the connection part. Preload of the spring can be adjusted to accommodate the roughness on the surface of the workpiece. Copper electrodes were bent to be able to stay close to the friction stir welding tool and therefore the stirring zone. Thin mica sheets were placed at the back of workpiece for insulation to avoid spread of electrical current into the backing plate. No insulation was placed on the tool based on the fact that electrical current will choose the shortest path to close the circuit. The relative position of two electrodes can be adjusted with the device shown in the left bottom corner of Fig. 1.  Fig. 1 CAD design of the experimental testbed adapted for electrically assisted friction stir welding Two types of electrode configurations have been investigated and are shown in Fig. 2. For Fig. 2(a), both of the electrodes were placed in the TRIP steel side and ideally only the steel side gets softening. The drawback is that the electrodes are a little far away from the tool pin and therefore only a small fraction of electrical current passes through the stirring zone. This can be improved in Fig. 2(b), where two electrodes span the different materials. The related problem is the uncertainty of the contact resistance at the abutting edge of the two workpiece. In order to attenuate this problem, the workpiece were clamped both vertically and laterally.

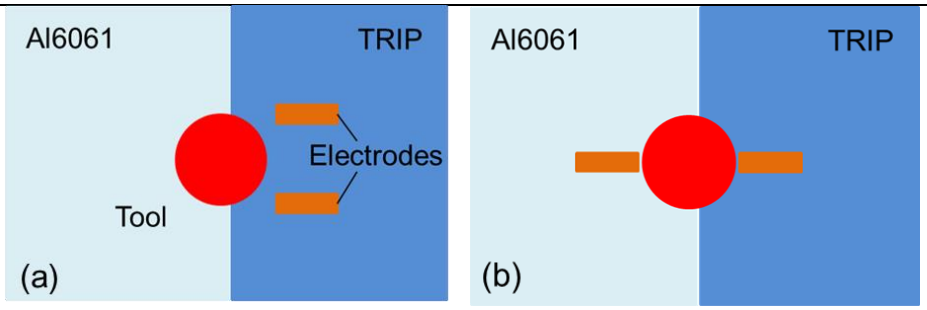


Fig. 2 Electrodes configuration

Electrical field distribution inside the workpiece was investigated using the finite element analysis software Abaqus 6.12. When an input current density of 18.78 A/mm^2 is applied at the electrodes, the current density in the center is around 17 A/mm^2, as shown in Fig. 3.

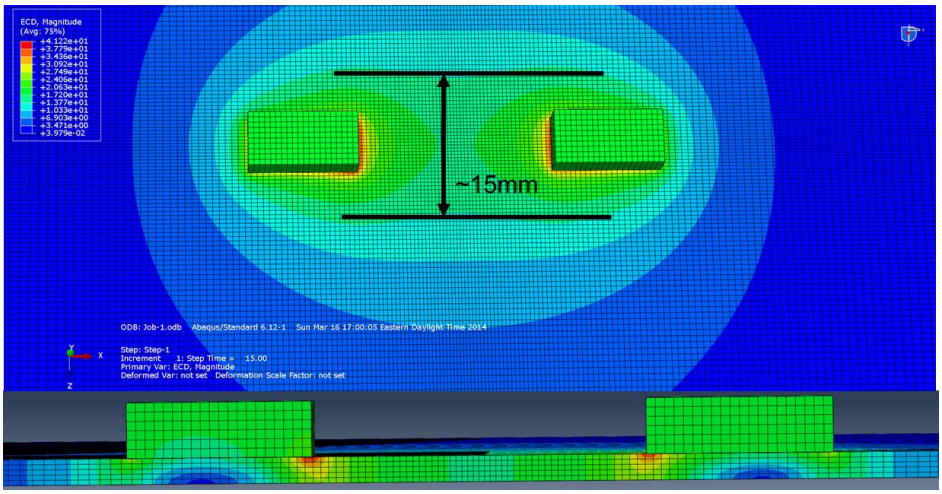


Fig. 3 FEA analysis result for the electrical current distribution in the workpiece

It can be further shown that the electrical field will not further distribute out when the length of the workpiece is larger than 50mm. Besides, higher input current density also hardly expand the electrical field, which is shown in Fig. 4 where a linear relationship between input current density and output current density can be observed.

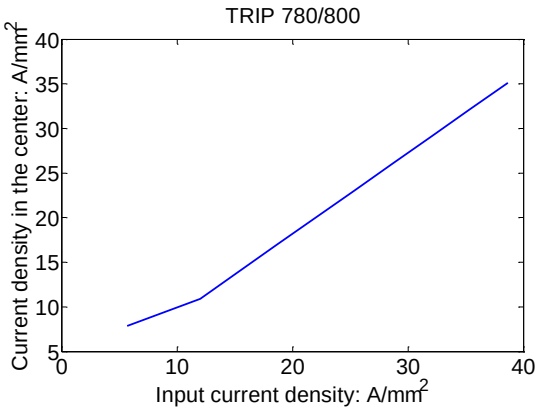


Fig.4 Relationship between input current density and output current density

Effect of electrical current was studied in the plunge stage of friction stir welding process for Al6061 and TRIP 780/800 respectively. The corresponding results on Al6061 are shown in Fig.5. It can be seen that both of the two peaks have been reduced.

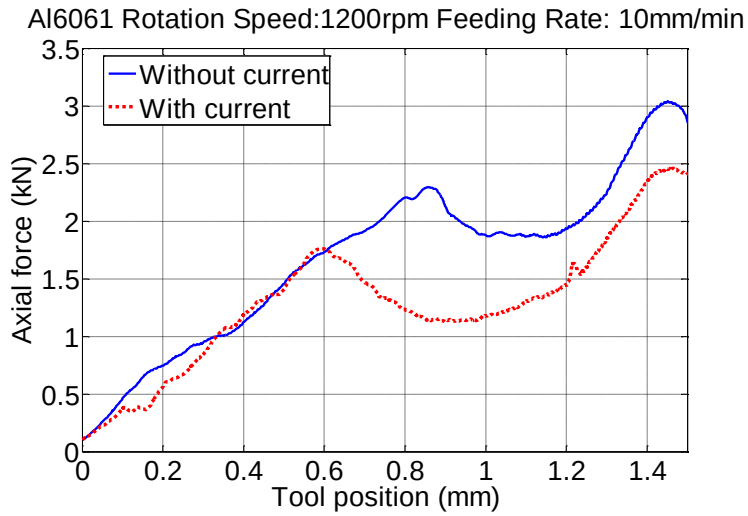


Fig. 5 Effect of electrical current on the plunge stage of Al 6061

When studying the electro-plastic effect for the plunge stage of TRIP 780/800 steel, certain temperature increase can be noticed. In order to identify the electro-plastic effect, the workpiece was further preheated with a slightly longer current period to reach a higher temperature before plunge. The axial welding force was then recorded and compared with other conditions. It can be seen in Fig. 5 that about 1/3 of the reduction of peak force comes from the thermal softening.

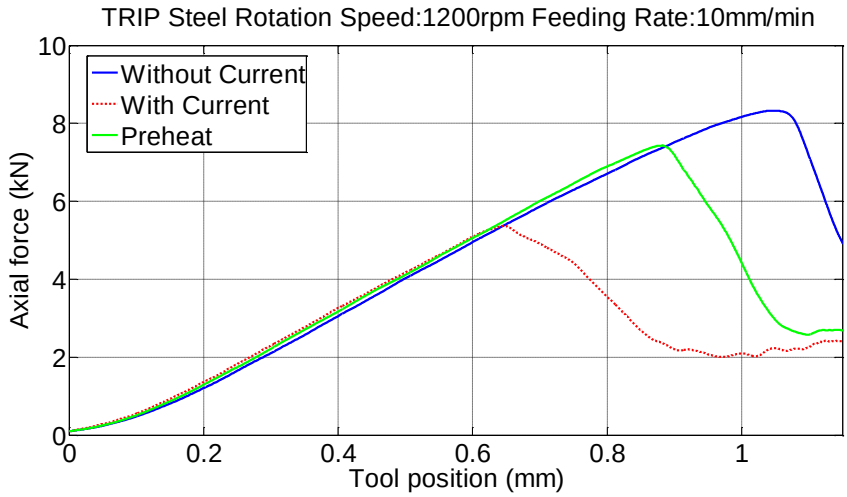
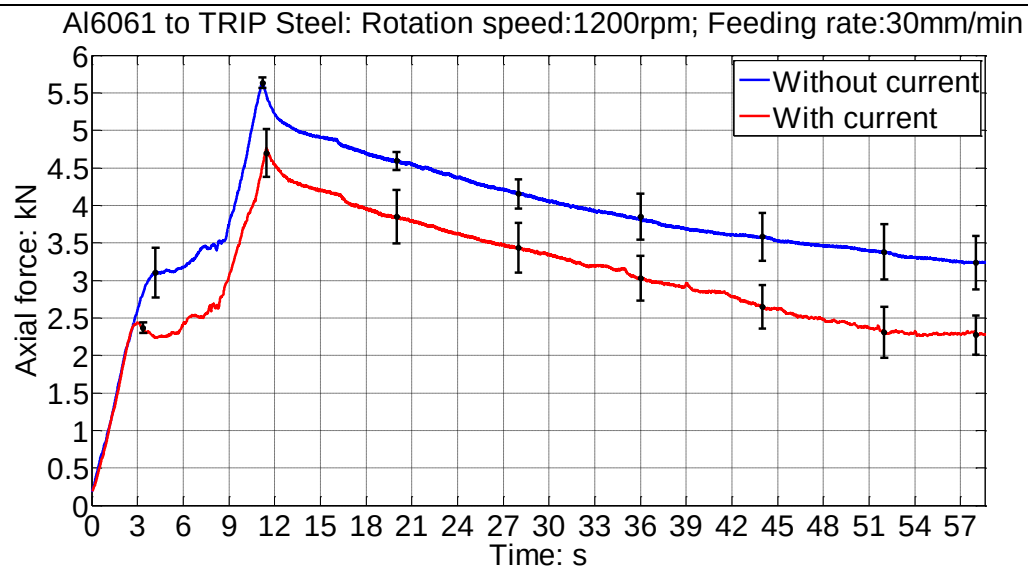
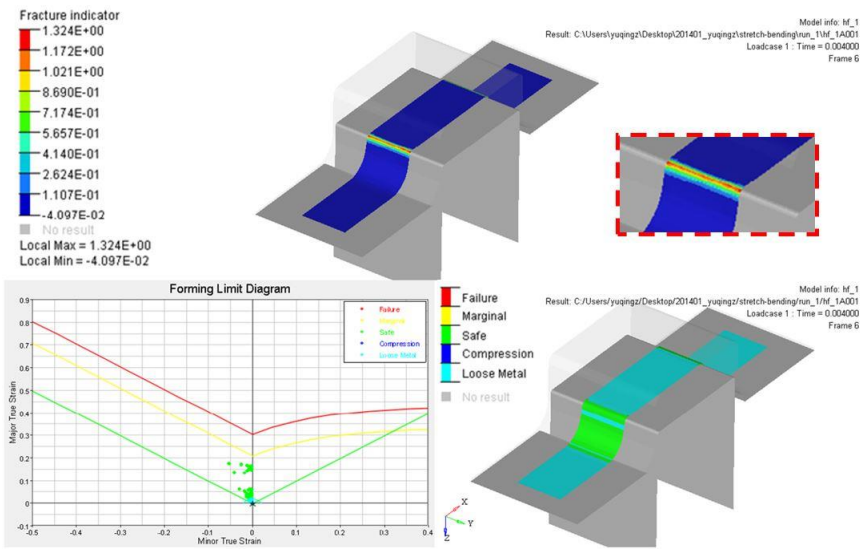


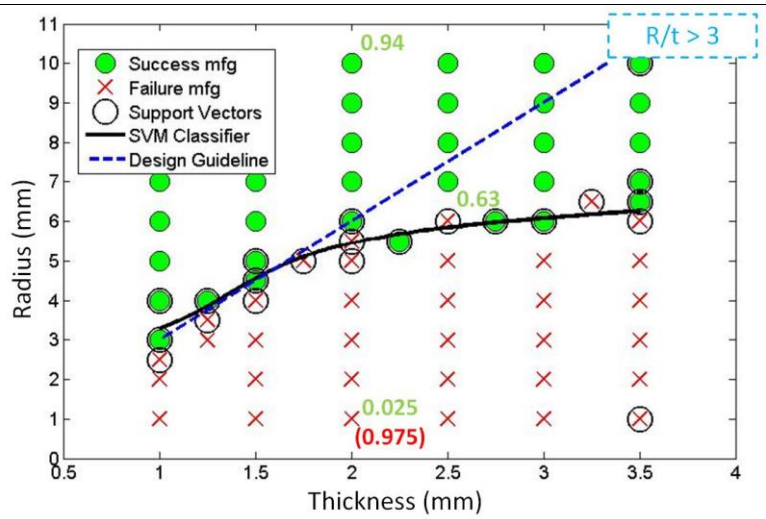
Fig. 5 Effect of electrical current on the plunge stage of TRIP 780/800 steel

Finally, the electrical current was applied in the whole friction stir welding process and the result is shown in Fig. 6. It can be observed that the axial force can be stably reduced.

	 Fig.6 Effect of electrical current on friction stir welding of Al6061 to TRIP 780/800
Industry Collaboration	A meeting with the Delphi friction stir welding team on April 8
US-China Collaboration Activities	N/A
Issues of Concern	• A numerical model describing FSW need to be established, which should account for recrystallization and intermetallic compound formation of steel and Aluminum. • A constitutive model incorporating electro-plastic effect need to be developed
Notable Recent Achievements	• Liu, X., Lan, S., & Ni, J. (2014). Analysis of process parameters effects on friction stir welding of dissimilar aluminum alloy to advanced high strength steel. Materials & Design, 59, 50-62. • Liu, X., Lan, S., & Ni, J. (2014). Experimental study of electrically assisted friction stir welding of dissimilar Al 6061 to TRIP 780/800 steel, MSEC 2014, Detroit, Michigan, USA

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	Mode-I Traction-separation laws for the initial adhesive identified by Eaton have been deduced from experiments conducted on DCB specimens. These were done by optically measuring the crack-opening displacement as a function of J-integral, and then backing out the traction separation law Mode-II specimens (lap-shear geometry) have been manufactured and tested. The analysis to deduce mode-II traction separation laws is on-going. This requires the use of ABAQUS to deduce the J-integral for the lap-shear geometry. If successful, this will provide a new technique to measure mode-II traction-separation laws. The mode-I results indicated that the adhesive identified by Eaton may be too brittle for their purposes. The toughness was only 200J/m^2, with a cohesive strength of 4 MPa. An additional set of different adhesives have been identified and sourced by Eaton. These have been delivered. Specimens will be manufactured with this adhesive and tested
Industry Collaboration	• Regular conference calls with Eaton • Site visit by Peter Fritz to UM in March 2014 to discuss use of new adhesives
US-China Collaboration Activities	• N/A
Issues of Concern	The original adhesive selected has been identified as being potentially too brittle for use in the desired applications. An additional set of adhesives has been identified, and will be tested.
Notable Recent Achievements	• N/A

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 activities by Chinese partners during this quarter. • Proposed active learning strategy for sequential efficient design of experiment which dramatically reduced the sampling computational cost; • Applied parallel computing on process simulations and massive sampling which dramatically saved data generation time; • Developed the simulation tool to accurately predict shear fracture for HSS/UHSS stretch-bending process;  • Applied the "manufacturability constraint modeling (MCM)" synthesis to UHSS (e.g. DP780) stretch-bending process for shear fracture failure mode on the tight radii critical feature; • Obtained the (R - radius, t - thickness) manufacturability constraint for DP780 stretch-bending process.

	
Industry Collaboration	Had discussion with Johnson Control on HSS/UHSS sheet stamping for their seat frames.
US-China Collaboration Activities	Continued to interact with SJTU team to compile DFM constraints for HSS/UHSS 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	• Extended the current constraint modeling method to another lightweight material manufacturing process; • The progress up to Dec 2013 was documented in a conference paper: Zhou, Y., and Saitou, K., "Identification of Manufacturability Constraints through Process Simulation and Data Mining", *Proceedings of the ASME 2014 International Design Engineering Technical Conference*, Buffalo, Aug 17-20, 2014, DETC2014-34542 (accepted)

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 submitted for publication in *Energy* • Finalizing econometric modeling to study spatial effects on PEV adoption within the state of Ohio using census tract-level data • Beginning more spatially detailed modeling of central Ohio at the street level • Applied for research grant from Google to geocode central Ohio vehicle registration data • Preliminary work examining distribution-level effects of level-3 fast PEV charging stations • Converted origin/destination tour record data for central Ohio into travel paths using shortest path problem • Determining optimal charging station locations using a flow-catching model • Converting PEV travel data into charging station demands • Combining charging station demands with building demands to model aggregate distribution-level load impacts
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 • 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, "Using Price-Based Signals to Control Plug-in Electric Vehicle Charging," forthcoming in *IEEE Transactions on Smart Grid*. • X. Xi and R. Sioshansi, "Wind Integration Benefits of Plug-in Electric Vehicles," submitted to *Energy*.

Thrust	TA 5: Vehicle-Grid Integration
Title	**Project 3: Control strategies for vehicle-grid integration (Joint)**
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	• Examined the ability of a large PEV fleet to achieve large-scale transmission objectives (valley filling, demand dispatch, regulation) while adhering to local distribution-level constraints (transformer overload, voltage quality) • Developed cohesive control strategy that achieves higher level objectives without damaging the grid • Analytically describing the limits of PEV control in this setting
Industry Collaboration	Ongoing discussions with Eaton on a proposed project for increased industry collaboration
US-China Collaboration Activities	Participated in web-based meetings with US and Chinese collaborators.
Issues of Concern	
Notable Recent Achievements	Awaiting decision on a conference paper on distribution level PEV charging coordination

Thrust Area 6: Energy Systems Analysis, Technology Roadmaps, and Policy

Thrust	TA 6: Energy Systems Analysis, Technology Roadmaps
Title	**Project 1: Life Cycle Assessment of Wireless Charging of Electric Vehicles (Joint)**
Personnel	PI: Gregory Keoleian (UM) Research Specialist: Robb De Kleine (UM) Graduate students: Zicheng (Kevin) Bi (UM) Visiting scholar: Lingjun Song (Beihang University)
Objective	• Compare the environmental performance of wireless charging to plug-in charging of electric vehicles using life cycle assessment • Conduct life cycle inventory analysis of both wired and wireless charging hardware • Develop a model to assess the environmental, energy, and economic benefits of wireless charging including potential lightweighting benefits from battery size reduction for fixed route vehicles such as transit buses
Progress Report	*January 2014* • Completed life cycle inventory of the wireless charger (material and manufacturing processes) and initial life cycle impact assessment of wireless charger in terms of Global Warming Potential and Cumulative Energy Demand *February 2014* • Built an initial model for comparison of wireless charging and plug-in charging, using Ann Arbor area bus system as a case study. *March 2014* • Attended the 2014 Wireless Power Transfer Workshop in UM Dearborn sponsored by IEEE, ANSYS, and the GATE Center for Electric Drive Transportation and received feedback from colleagues on our initial results. • Modified and added more complexities into the model to make it more realistic and potentially helpful for real-world decision making. Complexities added include different amounts of time of charging at each charging station in downtown and suburb, optimized distribution of wireless charging stations and different bus operation during weekday and weekend, etc.
Industry Collaboration	• Discussed the preliminary results with academic and industrial colleagues in the Wireless Power Transfer Workshop in UM Dearborn: Prof. Chris Mi (UM Dearborn), Prof. Chun Rim (KAIST, Korea)
US-China Collaboration Activities	• UM members worked directly with visiting scholar from Beihang University, China on gathering data and development of life cycle models
Issues of Concern	• None this quarter
Notable Recent Achievements	• Created a life cycle model to represent the material and manufacturing burdens of producing plug-in and wireless chargers (each charging system contains about 1000 components)

Thrust	TA 6: Energy Systems Analysis, Technology Roadmapping, and Policy
Title	**Project 2.1: Parametric Analysis of Clean Vehicle and Fuel Deployment in the Light Duty Transportation Sector (Cooperative US)**
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	• Incorporated data and model enhancements that account for real world driving behavior based on industry input. Completed initial analyses that consider impact of range penalties on BEV drivers. The model considers the difference between cost penalties versus thresholds for frequency of inconvenience for insufficient range. Analyses show willingness to adopt EVs for a breadth of battery ranges and driver characteristics. • Presented model and analysis results to TA6 partners in March monthly web meeting.
Industry Collaboration	• Reviewed preliminary model results with industry partners.
US-China Collaboration Activities	
Issues of Concern	• None
Notable Recent Achievements	• Initial results incorporating model enhancements with more realistic driving patterns completed and reviewed with industry partners and DOE.

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 (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	January: Finished sensitivity analysis 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). Refined regional optimal fueling strategy analysis based on sensitivity results. February: Conducted capacity analysis to assess the land requirement of using locally produced renewable energy to support transportation at the state level. March: Manuscript titled "Assessing Land Use Impact by Clean Vehicle Systems" in revision.
Industry Collaboration	• In contact with Microsoft Research Asia and Accenture China for potential collaborations
US-China Collaboration Activities	• Attended TA6 CERC Web-Ex Meetings
Issues of Concern	None to date
Notable Recent Achievements	• Manuscript titled "Assessing Land Use Impact by Clean Vehicle Systems" in revision.

Thrust	TA 6: Energy Systems Analysis, Technology Roadmaps & Policy
Title	**Project 4.1: Fleet Modeling on China's Alternative Fuels. (Cooperative US)**
Personnel	PIs: John Heywood (MIT) Graduate student: Summer Jiakun Zhao (MIT)
Objective	• Finalize the comparison of the three China studies and models including FLEET (MIT), EPPA (Emissions Prediction and Policy Analysis, MIT), and TCAEM (Tsinghua China Automotive Energy Model). • Conduct the comparison of the results and underlying assumptions for the these three models and studies; draft a journal paper prepared for publication. • Analyze the future growth of electric vehicles (including BEV, HEV and PHEV) in terms of stock and energy consumption in China. • Model the development of electric grid systems in China to forecast the electricity supply mix, in order to project the CO2 emissions associated with electric vehicles.
Progress Report	• January: Finalized the comparison of results and four key assumptions from the three studies. • February: Applied the FLEET model's fuel consumption improvement assumption (energy economy constraint values) to the EPPA model, which changed the EPPA energy consumption curve in the way that indicates how important the fuel economy assumption is to drive the result. Presented comparison results and findings to the sponsors. • March: Conducted research on the policies and current conditions of EVs, PHEVs, and HEVs, including policy targets, incentive programs, subsidies, barriers/challenges, charging infrastructures, consumer perceptions, and the involvement of state-owned enterprises.
Industry Collaboration	N/A
US-China Collaboration Activities	• January: Interacted with Professor Xunming Ou and graduate students from the Tsinghua University to discuss the underlying assumptions for the TCAEM model. • February: Presented the comparison results and findings at the Future Vehicles and Fuels Workshop on February 27, 2014. • March: Revisited the Sinopec USA office and interviewed the employees who shared insights of their views on the future development of electric vehicles.
Issues of Concern	The different level of details from the models makes the comparison difficult to perform; it is particularly not easy to find out the reason behind the different CO2 emission projections.
Notable Recent Achievements	N/A

Thrust	Thrust 6. Energy Systems Analysis, Technology Roadmaps and Policy
Title	**Project 4.2: Clean Vehicle Technology Roadmap and Policy Recommendations (Cooperative US)**
Personnel	PI: John 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	The current phase of work on this project expands on the results previously reported and published in recent journal articles. This ongoing work involves deconstructing the lifecycle-based Fuel Cycle Analysis (FCA) methods that have been commonly used for CVFS studies. It explains the issues that arise due to the static (equilibrium) nature of the models that underpin FCA methods when they are applied to inherently dynamic systems such as the carbon stock and flow interactions involves when using biofuels. Peer review comments on a draft paper, "The Liquid Carbon Challenge: Evolving Views on Transportation Fuels and Climate," were received in late March from the journal to which it was submitted and revisions are now underway. A final version will be completed early in the 2nd quarter and it is expected that publication will follow shortly thereafter. Also during this past quarter, several briefings and presentations were given on the work and its findings, including a presentation at the SAE Government-Industry Meeting in Washington, DC, and a seminar at Duke University. Outreach to CERC-CVC industry partners and other automotive and energy firms was also conducted, and planning is underway to host a small topical meeting involving technical experts from government, national laboratories, industry and academia to further discuss the implications of this work and identify future research needs.
Industry Collaboration	Although this work did not yet involve direct industry collaboration, substantive comments on the work in progress were received from CERC industry partners and others in the auto and energy industries.
US-China Collaboration	No direct collaborations underway.
Issues of Concern	None.
Notable Recent Achievements	Presentation of recent results at an SAE meeting and Duke University.

Thrust	TA 6: Energy Systems Analysis, Technology Roadmaps
Title	**Project 5: Assessment of automotive aluminum recycling infrastructure and allocation methods (Cooperative US)**
Personnel	PIs: Gregory Keoleian (UM) Research Specialist: Robert De. Kleine (UM) Graduate students: Arman Golrokhian (UM)
Objective	• Evaluate the importance of recycling allocation methods on vehicle's total life cycle. The magnitude and timing of emission vary significantly among different allocation methods. GHG and energy savings from lightweighting with aluminum can be considerably dependent on recycling allocation method. • Evaluate aluminum vehicle recycling processes and infrastructure to enhance the recycling of wrought aluminum components back into wrought aluminum vs. cast aluminum and avoid down cycling. The environmental benefits of avoiding degradation of recycled aluminum will be quantified.
Progress Report	January 2014 • Presented the results to CERC Trust 6 members via webinar on Jan 17th. • Completed the model for comparing *recycled content* and *end of life recycling* methods in the case of aluminum vehicle hood. February 2014 • Presented the primary recycling allocation results to EPA office in Ann Arbor NVFEL (National Vehicle & Fuel Emissions Laboratory) and modified the research question based on the feedbacks and existing area of concern. • Defined the boundaries of aluminum flow diagram in the case of vehicle lightweighting. March- April 2014 • Collecting data on current recycling infrastructure and sourcing of aluminum alloys from industry sources.
Industry Collaboration	Presented the primary results at EPA National Vehicle & Fuel Emissions Laboratory (NVFEL) on Feb-19th.
US-China Collaboration Activities	None this quarter
Issues of Concern	None this quarter
Notable Recent Achievements	Completed the model for comparing *recycled content* and *end of life recycling* methods in the case of aluminum vehicle hood.