CERC-CVC: U.S. - China Clean Energy Research Center Clean Vehicles Consortium
DE-PI0000012

Progress Report October 1st – December 31st 2013

A consortium lead by

The University of Michigan and Tsinghua University

in partnership with

Huei Peng

U.S. Director for CERC-CVC

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Executive Summary

Project Management Highlights

DOE Technical Review Meeting

DOE hosted a technical review of the CERC-CVC with VTP team lead participants from each of the corresponding technical areas. CERC-CVC leadership as well as thrust area leaders, site directors and industrial advisory board members were in attendance. All six thrust area leaders attended the meeting and presented the major achievements of the thrust areas. A formal report was received by CERC-CVC in early December, which is under review. Key points included the need to increase industrial involvement and the establishment of a document describing key outcomes. CERC-CVC leadership will address each point of feedback in the first quarter of 2014.

Project Scope

As a result of the feedback from the Executive Committee meeting in January, the CERC-CVC has grouped research projects in an effort to focus resources and increase collaboration. We have further consolidated projects in the biofuels and combustion area to combine the technically related tasks into projects. CERC-CVC now has 24 projects; 16 joint, 5 US Cooperative and 3 Chinese Cooperative. We continue to seek closer collaboration by coordinating the research efforts conducted by project teams in US and China.

Within this consolidated project model, we seek to concentrate our focus in key areas of interest to our industrial partners. In order to achieve this, the CERC-CVC US industrial partners have requested a review of the implementation pathways for all US based tasks. These pathways highlight the commercialization potential of each project and the barriers for achieving the next steps in the TRL progression. The next Industrial Advisory Board meeting in February of 2014 will review and select several of the projects for closer collaboration.

Collaboration

- Monthly Thrust Area Web Ex meetings are running regularly and schedules for 2014 are in development
- Battery researcher Jinichi Naruse from CERC Industrial Partner Denso Corp. joined Prof. Siegel's lab as a visiting scientist for a 18-month term beginning in November
- MIT Researchers are collaborating with scientists at Liox Power (Pasadena, California) on examining solvent effects on Li-O_2 redox reactions.
- Prof. Hofmann's finite element codes are being used by a postdoctoral student, Zifu Wang, on a separately-sponsored project funded by DENSO, a CERC member.
- OSU researchers are currently seeking partnerships with industrial collaborators including JAC in Hefei, Anhui, China to find vehicle applications of their fault diagnosis methods.
- Eaton is working with the hybrid bonding interface team to identify bonding modes of interest for increased collaboration.
- EP and FirstEnergy are actively involved in helping to explore power system and distribution-level effects of level-3 charging.
- AEP and FirstEnergy have expressed interest in also examining optimization of deployment of level-3 charging infrastructure, which would build off of work done examining levels-1 and -2 charging.

- MIT researchers are connecting with TU researchers exchanging and discussing comparison results between FLEET and TCAEM models in order to improve the models.

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. Periods 3, 4 & 5 have been shifted by 6 months, adjusting for initial delays in the contracting phase of the program. The partial funding of year three also caused some delays in expenditures due to the delayed contracting for the remainder of the budget. The program will now resume the originally scheduled cadence of research and spending. Significant cost share will be spent in the next 12 months to establish 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, 2 & 3	Budgeted	Actual
DOE	$ 7,500,000	$ 6,272,394
Cost-share	$ 10,989,052	$ 6,080,869
Total	$18,489,052	$12,353,263

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

- Dr. Nitin Kumar was awarded "Outstanding Poster Runner-Up" in the Postdoctoral Technical Showcase at Sandia in December 2013.
- Professor Siegel wins NSF CAREER award
- NAE Gilbreth Lecturer (Siegel)
- R.S. Goldman elected Fellow of the American Physical Society
- J.C. Walrath awarded National Science Foundation Graduate Research Fellowship
- Best Student Paper Finalist, Dynamic Systems and Control Conference, Palo Alto, CA, 2013. X. Zhou, T. Ersal, J. L. Stein, and D. S. Bernstein, "Battery health diagnostics using retrospective-cost system identification: Sensitivity to noise and initialization errors"

Advanced Batteries and Energy Conversion

Ramdon, S., Bhushan, B. and Nagpure S. C., "In situ Electrochemical Studies on Lithium-ion Battery Cathodes Using Atomic Force Microscopy," *J. Power Sources* (in review)

Wang, H., Liu, D., Co, A., Canova, M., Cao, L., and Downing, G., "Profiling Lithium Distribution in Sn Anodes of Lithium-Ion Batteries with Neutrons," submitted, *Journal of Radioanalytical and Nuclear Chemistry*.

Thermophysical Properties of $LiFePO_4$ Cathodes with Carbonized Pitch Coatings and Organic Binders: Experiments and First-Principles Modeling, Jagjit Nanda, Surendra K. Martha, Wallace. D. Porter, Hsin Wang, Nancy J. Dudney, Maxwell D. Radin, and Donald J. Siegel, Journal of Power Sources 251, 8-15 (2014).

David G. Kwabi, Betar M. Gallant, Jigang Zhou and Yang Shao-Horn, "Mechanistic studies of lithium-oxygen reactions using rotating ring disk electrode," Presented at Materials Research Society Fall Meeting; December 1 – 6, 2013; Boston, MA

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

Reaction Pathways for the Thermal Decomposition of Methyl Butanoate
Mohamad Akbar Ali and Angela Violi, *Journal of Organic Chemistry* 78(12), pp. 5898-5908 (2013)

Ab Initio/DFT Investigation of the Thermal Decomposition of n-Butylcyclohexane; Mohamad Akbar Ali, V. Tyler Dillstrom, Jason Y. W. Lai and Angela Violi (Accepted – Journal of Physical Chemistry A).

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 (in press), 2014.

Vehicle Electrification

Xiaowu Zhang, Huei Peng, Jing Sun, "A Near-Optimal Power Management Strategy for Rapid Component Sizing of Power Split Hybrid Vehicles with Multiple Operating Modes", 2013 American Control Conference, Washington DC.

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.*

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*.

Advanced Lightweight Materials and Structures

Zhao, Ziwei, Na Zhang, Yunior Hoie, L. James Lee, and Jose M. Castro. "Properties and process ability of long fiber-reinforced polymeric composites." Polymer Composites (2013).

"Vaporizing Foil Actuator: Controlling the Pressure Pulse for Impulse Metalwroking", S. R. Hansen, A. Vivek and G. S. Daehn, Submitted to Proceedings of the 2014 ASME Manufacturing Science and Engineering Conference, June 9-13, 2014, University of Michigan, USA. (Submitted)

"High Strain Rate Metalworking with Vaporizing Foil Actuator: Control of Flyer Velocity by Varying Input Energy and Foil Thickness"", A. Vivek, S. R. Hansen and G. S. Daehn, *Review of Scientific Instruments* (Submitted)

"Vaporizing Foil Actuators: A Tool for Collision Welding", A. Vivek, S. R. Hansen, B. C. Liu, G. S. Daehn, *Journal Materials Process Technology,* **213**, pp. 2304-2311 (2013).

X. Liu, S. Lan, J. Ni "Friction stir welding of dissimilar aluminum alloys to advanced high strength steel," Journal of Materials Processing Technology (under review)

X. Liu, S. Lan, J. Ni "Comprehensive analysis on the effects of process parameters on friction stir welding of dissimilar aluminum alloy to advanced high strength steel," Materials & Design (submitted)

"Identification of Manufacturability Constraints through Process Simulation and Data Mining" to be submitted to ASME Design for Manufacturing and the Life Cycle conference to be held in August 2014.

Vehicle-Grid Integration

None this period

Energy Systems Analysis, Technology Roadmaps and Policy

DeCicco, "The Liquid Carbon Challenge: Evolving Views on Transportation Fuels and Climate," was prepared and submitted to a journal for peer-review

Cai, H.; Xu, M. Greenhouse gas implications of fleet electrification based on Big Data-informed individual travel patterns. Environmental Science & Technology 2013, 47 (16), 9035-9043

DeCicco, "Biofuels carbon balance: doubts, certainties and implications", *Climatic Change* (online, Sept. 2013), http://dx.doi.org/10.1007/s10584-013-0927-9

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. The first images were collected from the Li-wire half-cell using in-situ electrochemical atomic force microscopy (AFM). While the charge and discharge characteristics of the Li-wire half-cell do not completely follow those of a commercially available $LiFePO_4$, the AFM image analysis was able to quantify particle area changes during battery cycling, a unique diagnostic capability. Significant process was also made in the design and assembly of an in-situ electrochemical cell for X-Ray diffraction. Initial results have been obtained from the half-cell prototype for in-situ neutron depth profiling (NDP), collecting several spectra during charging and discharging of the cell to grow the understanding of the lithiation and delithiation of a Sn anode. The atomic scale modeling work continues to study the interaction between electrolyte and cathode to engineer electrode surfaces that minimize electrolyte oxidation. Preliminary results show that, when the battery is nearly halfway to charge/discharge state, complete decomposition of ethylene carbonate (EC), a prime organic electrolyte for LIBs becomes viable. Work on future battery chemistries such as Li-air and Na-air systems also continues at UM and MIT.

In the biofuels and APU thrust, important fundamental work continues to model novel biofuel molecules. The work on modeling 2,5-Dimethylhexane, a key component of bisabolene, continues with the modeling of the low temperature oxidation of the secondary radical. The resulting reaction rates were input back into the base alkane models with the modified reaction mechanisms to simulate the oxidation in a shock tube. Further rates of high and low temperature combustion pathways and shock tube simulations have been performed, with the goal of one model that will characterize a wide range of combustion temperatures and pressures. The team continues to investigate suitable fuels for experimental testing in a shock tube to verify the combustion model and also share with colleagues in China. Powertrain efficiency gains post engine in the area of thermo electrics focused on studying inhomogeneity of thermoelectric

materials. Using scanning tunneling electron microscope techniques large variations from the mean of the Seebeck coefficient were found in bulk skutterudite polycrystalline samples. Similar techniques showed uniform density of states and Seebeck coefficient across the scanned surface of single crystal samples of bulp p-GaAs and bulk Sb_2Te_3.

In the electrification thrust, the finite element algorithm developed for electric machines are being extended to become applicable to asynchronous machines. 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 best configurations obtained from the Power-weighted Efficiency Analysis for Rapid Sizing (PEARS) method are being analyzed more closely for possible patent applications. Two configurations were shown to achieve roughly 7% better fuel economy compared with the Prius 2010 design. The research in to developing effective and robust system identification algorithms for on-line detection of battery state of health has focused on the possibility of efficient multi-cell battery system identification using support vector based model parametrization. This would alow for the development of a multi-cell battery model based on a model developed from single cell data, saving computational time, 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. Research at OSU showed nanoparticles were beneficial for enhancing the flexural performance of polymer composites, but further work is necessary to determine the optimal amount of nanoparticles. The new collision welding technique under development is moving to sample assemblies with two welds in series between the same two sheets, in an effort to create an aluminum-steel part containing multiple joints. The hybrid Friction Stir welding process incorporating electroplastic effects has finished development of an experimental setup and progress has been made on developing a finite element model for the novel process. At the vehicle level, researchers have demonstrated the data-mined design guidelines outperforming well-established design guidelines in terms of the binary prediction accuracy of stamping failures in parts with various geometries. In addition, an algorithm was developed to compute confidence values of the design guidelines identified through data mining. The tools were used to study how mass distribution of the battery and occupants would influence crash response in a mini-EV.

Electrification is not just promising for increased efficiency; it also allows vehicles to interface with the electric grid and possibly renewable energy sources. Pricing-based charging control strategies continue as well as economic modeling studying spatial effects on alternative vehicle adoption. Model enhancements that account for real world driving behavior are being incorporated in to the model. Also, the scope of technology and policy issues that can be addressed is being expanded, including the implementation of different models of consumer interpretation of range and public charging limitations and their influence on EV adoption. The controlled response of the grid to these PEV's continues with the development of a simulated three phase power flow solution algorithm that analyzes voltage dynamics and the effects on transformers. Work continues to understand, quantify, and reduce the oscillatory behavior that appears under certain circumstances.

Finally, work continues in thrust area 6, the energy systems analysis, technology roadmaps, and policy thrust. The vehicle design and assessment work has resulted in finalized life cycle results

for engine, material, and vehicle combinations, including the assessment of the impact of required structural support for electrified vehicles. With respect to biofuels, a parametric analysis of technology advancement and policy tradeoffs as they pertain to the Renewable Fuels Standard was completed, identifying the price differential with gasoline as the key barrier to increased adoption, and not the lack of refueling station availability. Model enhancements that account for real world driving behavior were also incorporated in to the model based on industry input. The fuel mix strategy team investigated the fleet level water consumption based on the Sandia National Laboratory fleet model, and conducted a sensitivity analysis for land impact of clean vehicles and assessed land constraints on production capacity of transportation fuels produced from wind, solar, and biofuel sources at the state level.

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) Post Doc: Dervis Emre Demirocak, Shrikant C. Nagpure (OSU) Students: Samartha Channagiri (OSU)
Objective	Improve the robustness of current-generation Li-ion Batteries via detailed characterization of degradation and aging mechanisms.
Progress Report	1. Aging Cells: The reinstallation and calibration of the cyclers in our new facility is underway. The initial characterization test to estimate the status and performance parameters such as capacity and internal resistance of the four cells that started last quarter will continue. 2. In-situ Electrochemical AFM: Morphological changes of $LiFePO_4$ cathode particles during cycling were investigated using the Li-wire cell design as shown in **Fig. 1**. To ensure proper operation of the Li-wire cell, cycling data from commercial $LiFePO_4$ cell was compared with the Li-wire cell. The charge and discharge curves of commercial and Li-wire cells at a C/6 rate are given in **Fig. 2** and **Fig. 3**, respectively. The commercial $LiFePO_4$ cell, **Fig. 2**, showed a flat voltage plateau (≈ 3.4 V) during dis-/charging due to two phase reaction between $FePO_4$ and $LiFePO_4$ as expected. However, Li-wire cell, **Fig. 3**, showed slight overpotential (≈ 3.6 V) and underpotential (≈ 3.3 V) during charging and discharging, respectively. This phenomenon is associated with the increased resistance within the in-situ half cell as compared to the commercial cell. In addition, due to electrolyte evaporation from in-situ cell, it was not possible to collect data during the whole charging or discharging cycle. Therefore, the charging cycle was stopped after 3 hours and the discharging of the in-situ cell was started as shown in **Fig. 3**. The AFM images were continuously collected during charging and discharging. The AFM images collected at three different instants (i.e., initial, at the end of charge and at the end of discharge) were analyzed to reveal the particle area changes during the cycling. The AFM images collected are given in **Fig. 4**. Initially, particle area was 0.3 μm^2, upon charging for 3 hours, particle area had decreased to 0.26 μm^2 (13 % decrease), upon discharging particle area had increased to 0.33 μm^2 (27 % increase). $LiFePO_4$ cathode particles are expected to show 6.8 % volume change between fully charged and discharged states as indicated in the literature. The surface area change we have found in this in-situ AFM study is considerably higher than the expected volume change indicating that $LiFePO_4$ particles are significantly contracting in the vertical (i.e., z) direction to match 6.8 % volume change. Further studies will focus on the design issues associated with the in-situ AFM cell and the analysis of $LiFePO_4$ particle size change during cycling utilizing numerous particles to draw statistically significant results. 3. In-situ X-Ray Diffraction: An in-situ electrochemical cell was assembled. The schematic of the cell is shown in **Fig. 5**. The design of the cell was tested for optimum XRD signal by finding the right z-position to obtain maximum X-ray diffracted intensity from the working electrode of the in-situ cell. The in-situ cell design is being optimized for the performance based on the results of this study. The subsequent XRD pattern obtained is shown in **Fig. 6**. Based on the outcome of this test, some modifications to the cell design such as working electrode diameter, source slit size and window material are being considered. A new cell

	is being built based on these considerations. 4. <u>Analysis of Standards:</u> The XRD patterns of pristine $LiFePO_4$ and $FePO_4$ samples are being obtained to establish a standard pattern for comparison with the pattern that will be obtained during the in-situ XRD study. Standard XRD spectra have been collected of pure $LiFePO_4$ powder (obtained from Sigma-Aldrich®) and indexed (**Fig. 7**). Pure $FePO_4$ was prepared from $LiFePO_4$ by chemical delithiation using NO_2BF_4 as an oxidizing agent. XRD of $FePO_4$ will be obtained and indexed in the coming quarter. After this, partially delithiated samples (Li_xFePO_4) (x=0 to1), will be analyzed using XRD. All of the above will be used to analyze the final XRD data from working electrodes of in-situ cells used.
Industry Collaboration	
US-China Collaboration Activities	
Issues of Concern	None
Notable Recent Achievements	Ramdon, S., Bhushan, B. and Nagpure S. C., "In situ Electrochemical Studies on Lithium-ion Battery Cathodes Using Atomic Force Microscopy," *J. Power Sources* (in review)

<u>Appendix:</u>

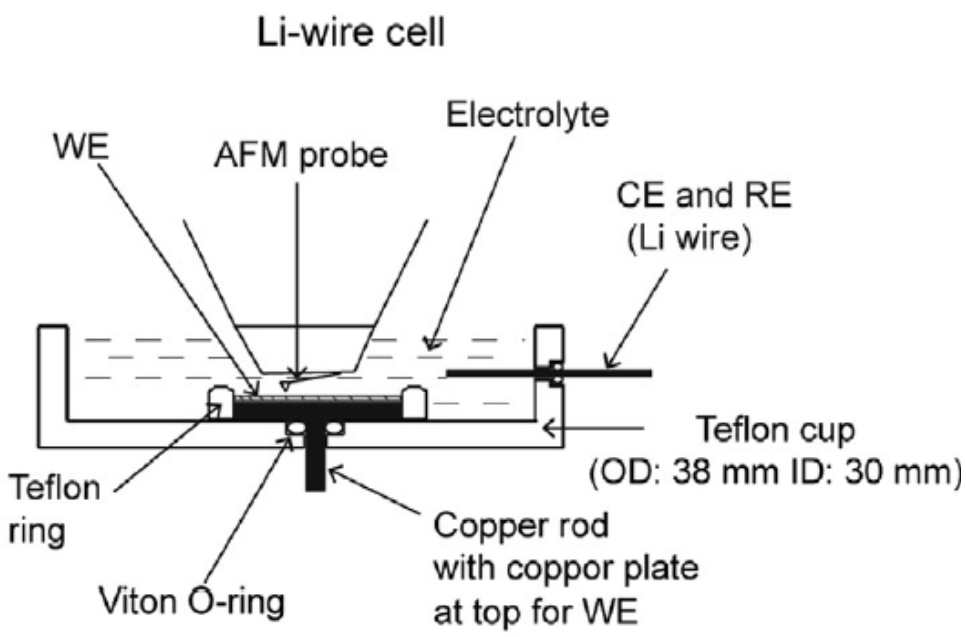


Figure 1: Li-wire cell design.

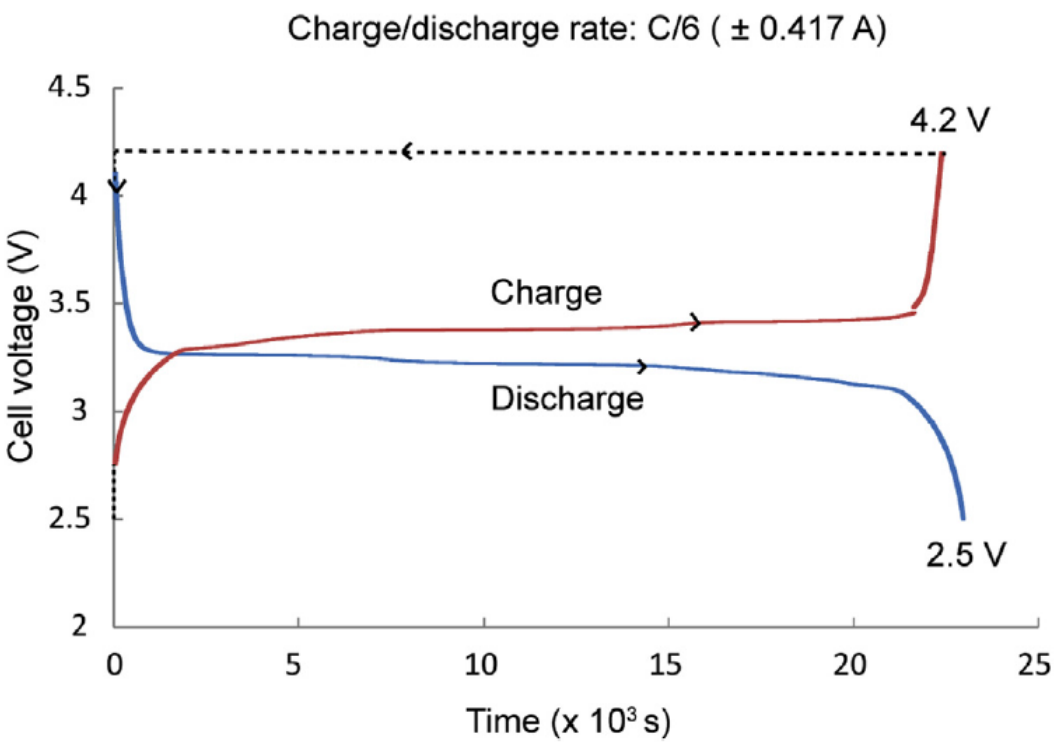


Figure 2: Charge and discharge curve of a commercial LiFePO4 cell.

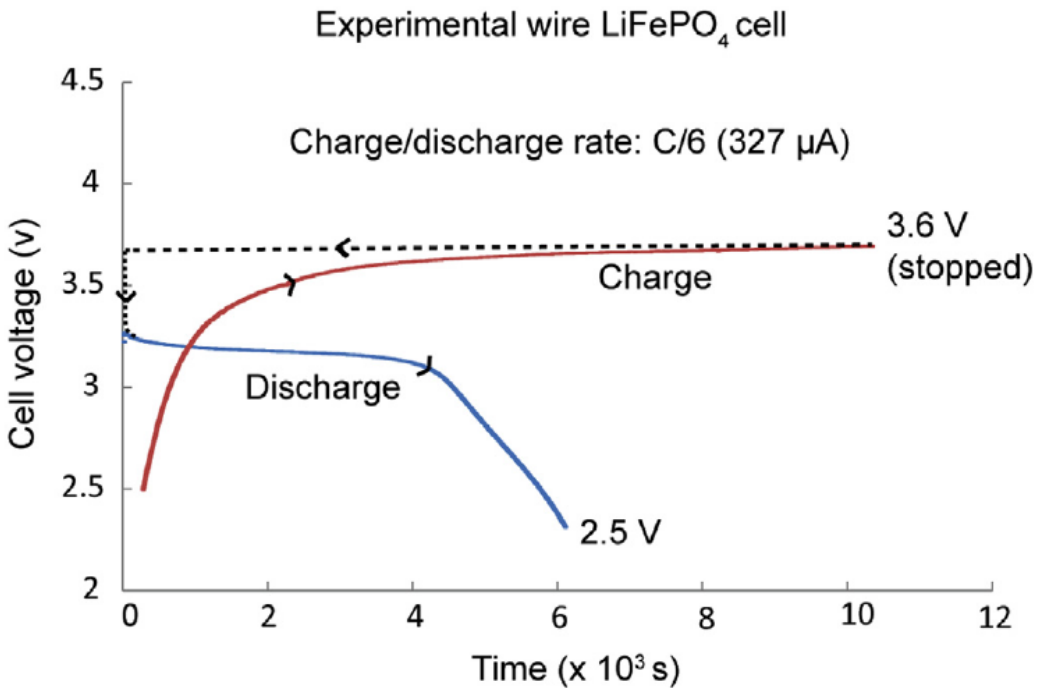


Figure 3: Charge and discharge curve of the Li-wire cell.

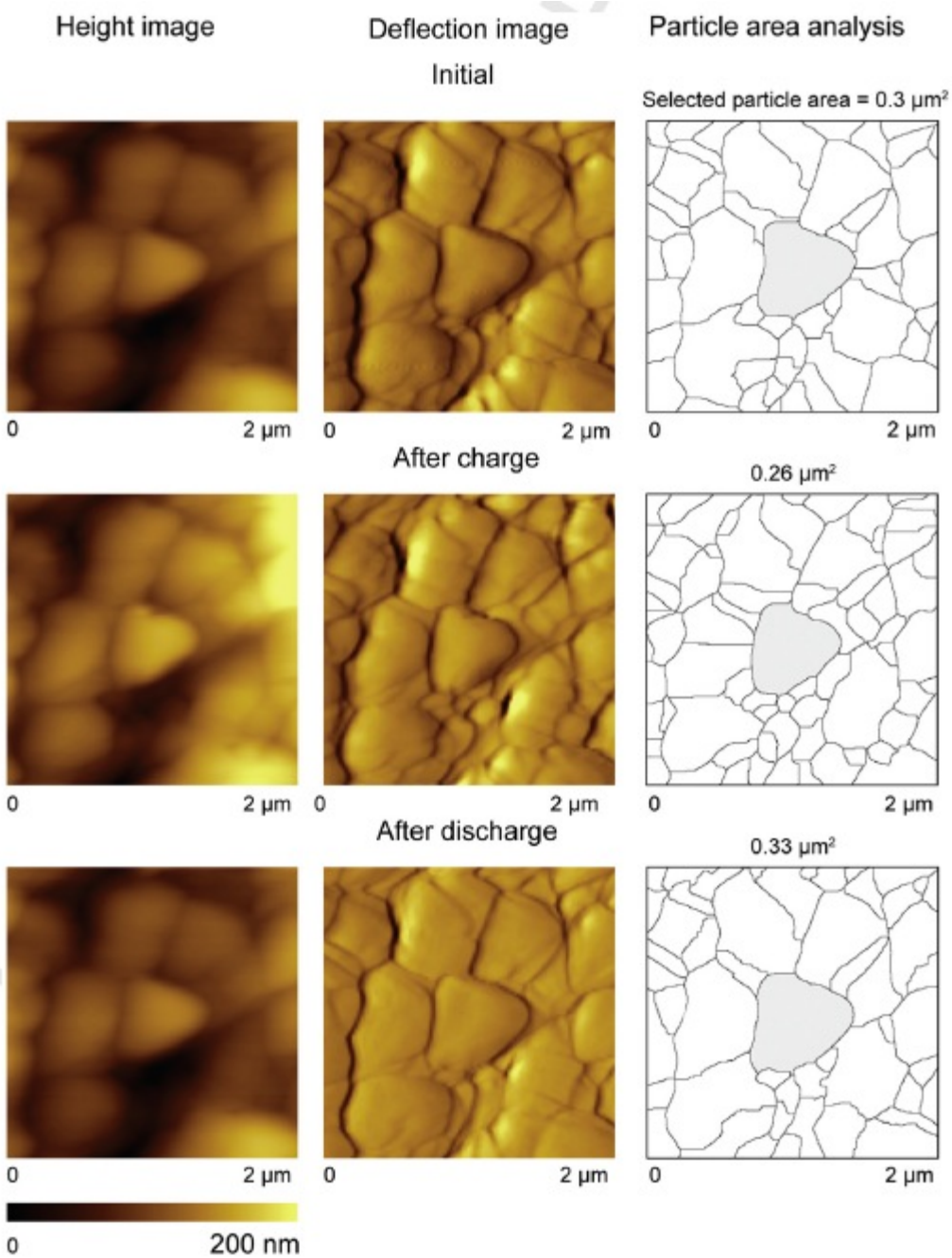


Figure 4: AFM height and deflection image as well as particle area analysis of LiFePO4 cathode showing change of particle size between charged and discharged states.

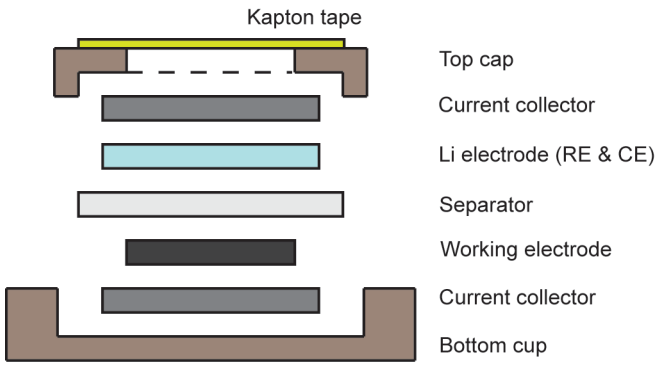


Figure 5: A schematic of in-situ XRD cell.

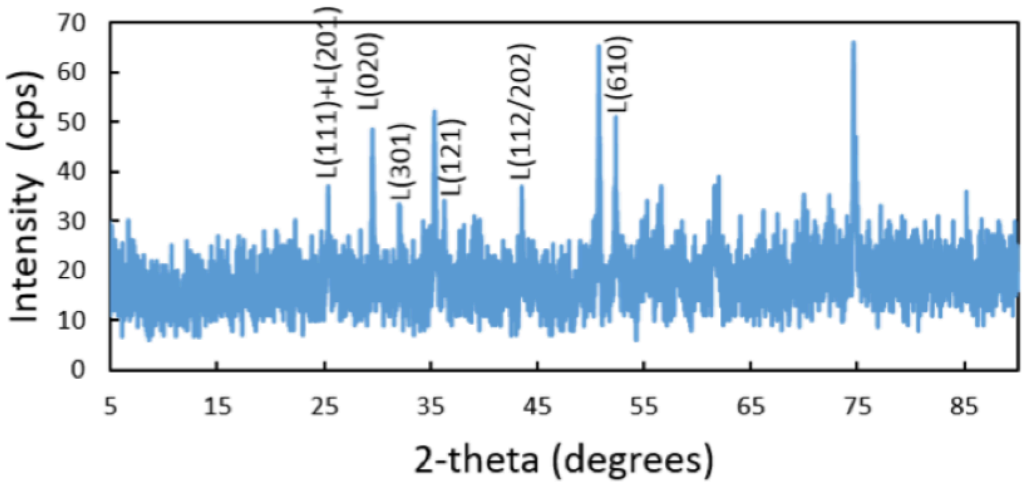


Figure 6: A representative XRD pattern obtained from the sample in in-situ cell.

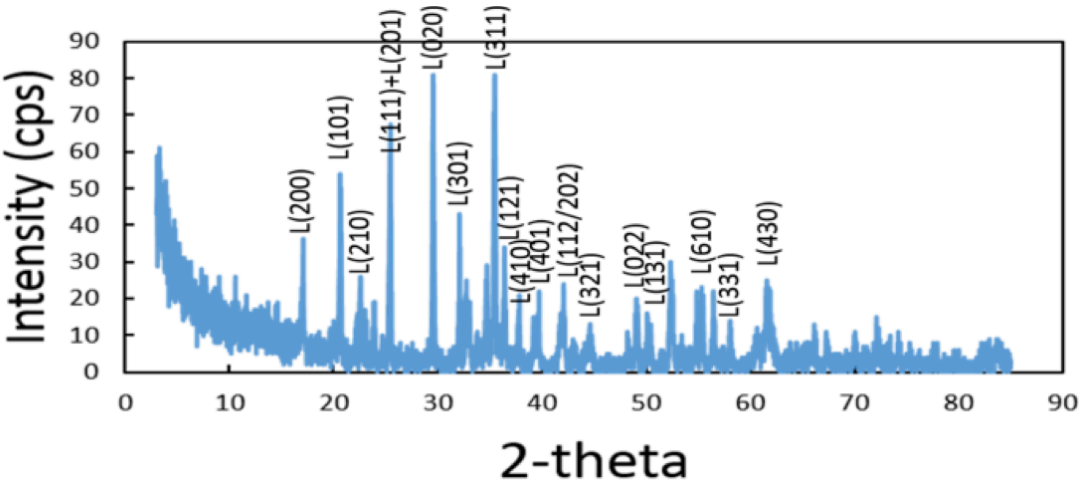


Figure 7: XRD pattern obtained as standard pattern by analyzing pure $LiFePO_4$ powder from Sigma-Aldrich®

Thrust	TA 1: Advanced Batteries and Energy Conversion
Title	**Project 1.2: In-situ Neutron Depth Profiling of Lithium Ion Battery Materials for Improved Electrochemical Performance and Aging Models (US Cooperative)**
Personnel	PIs: Marcello Canova (OSU), Raymond Cao (OSU), Ann Co (OSU) Post Doc Researcher: Shrikant C. Nagpure (OSU) Graduate Students: 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	1. <u>Half-cell Prototype for In-situ NDP</u>: This quarter we successfully demonstrated the *in situ* NDP measurement technique, by developing a design for an in-situ cell and building an experimental setup that allowed one to measure the Li concentration in the near-surface region of an Sn anode during cycling of the cell. The *in situ* cell prototypes were built at OSU and the NDP facility at the National Institute of Standards and Technology (NIST, Gaithersburg, MD, USA) was leveraged to measure the lithium concentration depth profile. The facility provides a well-collimated "cold" neutron (~5 meV) fluence rate of 7.6 $\times 10^8$ $cm^{-2}s^{-1}$ with a nominal beam area of 110 mm^2. 2. <u>NDP Analysis of Lithiated Sn Anode Samples:</u> An *in situ* measurement of an electrochemical cell to probe the dynamics of lithium migration was performed using our *in situ* cell setup. The results are shown in **Fig. 1**. The inset in the **Fig. 1** shows the schematic of cell geometry and the experimental setup. The Celgard™ separator is wetted with 1M $LiBF_4$ in EC:DMC (1:1 wt%) solution, the data were collected every 5 minutes for 5 hours. In **Fig. 1,** the black curve shows the initial lithium atoms in the wetted Celgard™ separator, the blue curve is a snapshot showing the lithium drifting into Sn anode when lithiation started, and the red curve shows the lithium at near-saturation conditions in the Sn with longer lithiation time. The right edge of the red spectrum clearly indicates the lithium ions have been driven throughout the Sn, reaching the interface between Sn and Kapton. This measurement shows the first *in situ* probing of lithium ions in the battery, when it is charged and discharged. The lithium dynamics as captured by charged particles provides invaluable information to our battery study. Several spectra have been collected during charging and discharging of the cell to understanding the lithiation and delithiation of Sn anode. These spectra will be analyzed in the coming quarter and the results will be summarized in a peer-reviewed publication.
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	• Wang, H., Liu, D., Co, A., Canova, M., Cao, L., and Downing, G., "Profiling Lithium Distribution in Sn Anodes of Lithium-Ion Batteries with Neutrons," submitted, *Journal of Radioanalytical and Nuclear Chemistry*.

Appendix:

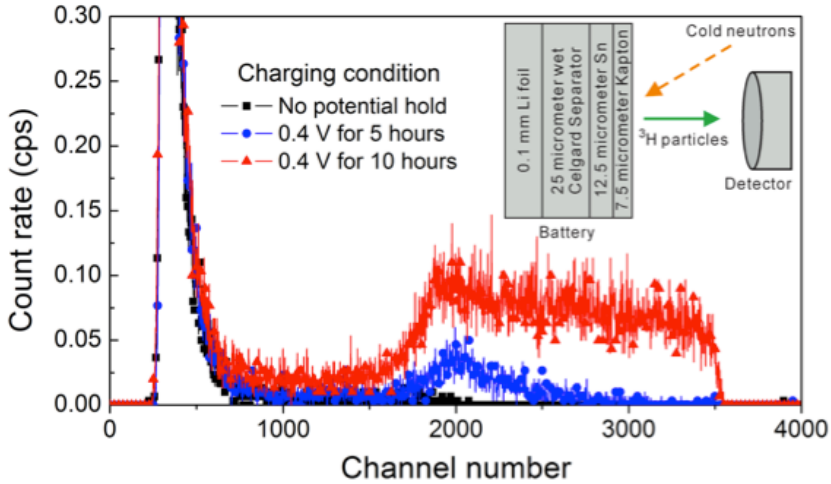
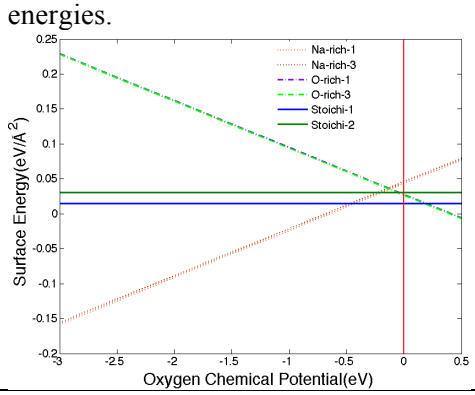


Figure 1. *In situ* NDP spectrum for a Sn-anode based lithium ion cell during charging

Thrust	TA 1: Batteries
Title	**Project 1.3: Li-ion battery aging and internal degradation mechanisms (US Cooperative)**
Personnel	PIs: Kevin Leung (Sandia), Don Siegel (UM), Post Doc: 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.
Progress Report	Rechargeable lithium-ion batteries (LIBs) are under intensive research for their use in energy storage and transportation applications, such as electric vehicles (EV). An economical, safer and environmentally friendly alternative to presently used Cobalt in cathode material is to replace it with Manganese. For this reason, $LiMn_2O_4$ (LMO) spinel and high voltage Ni substituted LMO are becoming promising cathode substitutes for LIBs[1]. However, one of the major challenges in the successful use of LMO is related to its vulnerability to electrolyte degradation which eventually results in capacity loss and poor cycling stability[2]. We recently showed[3] evidence for electrolyte decomposition on LMO (100) surface. The more common (111) surface of LMO was theoretically predicted[5] after our previous work[4] on (100) surface. Interestingly, the two surfaces are experimentally shown[6] to have significantly different electrochemical behavior with (111) surface forming a stable thin film of decomposed electrolyte. Hence, in the present work, we are modeling degradation mechanisms of ethylene carbonate (EC), a prime organic electrolyte for LIBs, on the prominent (111) facet of LMO cathode. A deeper understanding of interaction between electrolyte and cathode, especially with surface termination dependence, provides an opportunity to engineer electrode surfaces such that the electrolyte oxidation can be minimized. In our previous report, we showed that one of the possible EC decomposition route includes a two-step reaction. The first step is H-abstraction, where a proton from EC gets abstracted and ends up at one of the surface oxygens. The second step is the ring opening process where the EC's carbon-oxygen bond is broken. We found that the H-abstraction was the rate determining step. We have studied the effect of changing the Li content, which corresponds to changing the state of charge of the battery, on these two barriers. We find that when the battery is fully discharged, the H-abstraction barrier is more than 1 eV whereas the ring opening process is almost boundless. Interestingly, as the battery charges, the H-abstraction barrier decreases but the ring opening barrier increases. Preliminary results on our somewhat small slab model show that, when the the battery is nearly halfway to charge/discharge state, the two barriers are such that the complete decomposition of EC becomes viable. The reaction rate for the two reactions is estimated to be 10^2 and 10^6 reactions per second. In near future, we are planning to use the metadynamics technique to study further decomposition of EC. The presently gained knowledge will enable us to study electrolyte/electrode reactions for industrially relevant high voltage cathodes such as Ni substituted LMO. 1. Bruce, P. G., Scrosati, B. & Tarascon, J.-M. Nanomaterials for Rechargeable Lithium Batteries. *Angew. Chem. Int. Ed.* **47,** 2930–2946 (2008). 2. Hunter, J. C. Preparation of a new crystal form of manganese dioxide: λ-MnO2. *J. Solid State Chem.* **39,** 142–147 (1981). 3. Leung, K. First-Principles Modeling of the Initial Stages of Organic Solvent Decomposition on LixMn2O4(100) Surfaces. *J. Phys. Chem. C* **116,** 9852–9861

	(2012). 4. Huang, M.-R., Lin, C.-W. & Lu, H.-Y. Crystallographic facetting in solid-state reacted LiMn2O4 spinel powder. *Appl. Surf. Sci.* **177,** 103–113 (2001). 5. Karim, A., Fosse, S. & Persson, K. A. Surface structure and equilibrium particle shape of the LiMn2O4 spinel from first-principles calculations. *Phys. Rev. B* **87,** 075322 (2013). 6. Hirayama, M., Ido, H., Kim, K., Cho, W., Tamura, K., Mizuki, J. & Kanno, R., Dynamic Structural Changes at LiMn2O4/Electrolyte Interface during Lithium Battery Reaction. *J. Am. Chem. Soc.* **132,** 15268–15276 (2010).
Industry Collaboration	• We are actively seeking U.S. industrial partnership for potential interaction/collaboration. The fundamental understanding of electrolyte interaction with the cathode will enable us to apply the knowledge gained to a more industrially appropriate cathode material, such as Ni substituted LMO, and other potential organic electrolytes. In a recent review by industrial partners, one party expressed interest in potential collaboration after the end of this project.
US-China Collaboration Activities	• None
Issues of Concern	• None
Notable Recent Achievements	Dr. Nitin Kumar was awarded "Outstanding Poster Runner-Up" in the Postdoctoral Technical Showcase at Sandia in December 2013.

Thrust	TA 1: Advanced Batteries and Energy Conversion
Title	**Project 2.1: High Energy Density Battery Chemistries (Joint)**
Personnel	PIs: Don Siegel (UM), Anton Van der Ven (UM), Feng Wu (BIT), Borong Wu (BIT), Xiang-Ming He (THU) Graduate students: Alexandra Emly, Max Radin (UM) Visiting scholar: Xiankun Huang, PhD Student (THU)
Objective	• Identify of mechanisms that limit the performance of Li-air batteries, including: high charging potentials, poor reversibility, and limited capacity/capacity fade.
Progress Report	We are continuing our modeling of the discharge phases in Na-O2 batteries. In these batteries both Na_2O_2 and NaO_2 are found to be reversible in experiments, however systems that discharge NaO_2 (sodium superoxide) exhibit much lower overpotentials upon charging. As a first step towards understanding these results, the surfaces and conductivity of Na-O2 phases are being investigated using density functional theory and quasi particle calculations. Our preliminary calculations indicate that the bandgap for Na_2O_2 is 6.65eV, while for NaO_2 the bandgap is slightly smaller, 5.29 eV. These results suggest that both compounds will be somewhat poor intrinsic (band) conductors. To predict the morphology of discharge crystallites, we calculated the surface energies of 34 distinct Na_2O_2 surfaces and 16 unique NaO_2 surfaces. Van der Waals-augmented Density Functional Theory (vdw-DF2 functional) was used to account for dispersion interactions involving O2 units. (Conventional GGA-based functionals were found to give poor results for the surface energies.) A plot of surface energies for various NaO_2 (100) terminations as a function of oxygen chemical potential is shown in Figure 1. Different from Na_2O_2 surfaces, stoichiometric surfaces in NaO_2 have the lowest energies.  **Figure 1.** Surface energies for various NaO_2(100) surface terminations as a function of oxygen chemical potential. The red vertical line shows the oxygen rich limit. The surface having the lowest surface energy at 1 atm is plotted in blue.
Industry Collaboration	• Monthly teleconferences were held amongst U.S. researchers and industrial partners. • A new task to leverage the ORNL Battery Manufacturing Facility for battery degradation studies was discussed at the monthly telecons, and will involve collaboration between several Thrust participants. • Battery researcher Jinichi Naruse from CERC Industrial Partner Denso Corp. joined Siegel's lab as a visiting scientist for a 18-month term beginning in November.
US-China Collaboration Activities	
Issues of Concern	None.
Notable Recent Achievements	Paper published: • *Thermophysical Properties of $LiFePO_4$ Cathodes with Carbonized Pitch Coatings and Organic Binders: Experiments and First-Principles Modeling*, Jagjit Nanda,

	Surendra K. Martha, Wallace. D. Porter, Hsin Wang, Nancy J. Dudney, Maxwell D. Radin, and Donald J. Siegel, Journal of Power Sources 251, 8-15 (2014). Awards received: • NSF CAREER award (Siegel) • NAE Gilbreth Lecturer (Siegel)

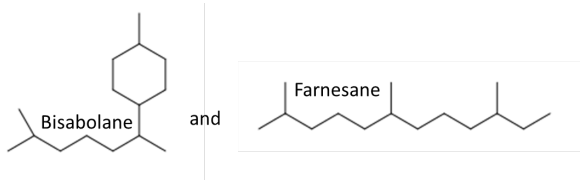
Thrust	TA 1: Advanced Batteries and Energy Conversion
Title	**Project 2.2: Fundamental Understanding of Li-Air Reaction Mechanisms (Joint)**
Personnel	PIs: Yang Shao-Horn (MIT), Gerbrand Ceder (MIT) Graduate students: David Kwabi (MIT), ShinYoung Kang (MIT)
Objective	Wide scale adoption of $Li-O_2$ batteries is currently hampered by device-level performance challenges such as low-roundtrip efficiency and poor cycle life. The objective of this project is to understand these limitations by studying fundamental reaction mechanisms in $Li-O_2$ cells. Specifically, we wish to: • Investigate morphology and crystallinity of $Li-O_2$ reaction products using electron microscopy. • Study the contribution of soluble oxygen reduction reaction (ORR) intermediate species (such as O_2^- and LiO_2) to Li_2O_2 growth, morphology and surface chemistry using rotating ring disk electrode (RRDE) measurements. • Characterize spatial distribution of distinct species in discharge product via nanoscale chemical imaging with the Scanning Transmission X-ray Microscopy technique. • Computationally investigate the reaction paths and energies between LiO_2, the possible intermediate phase during charging, with electrolyte.
Progress Report	• RRDE measurements have been used to detect the existence of soluble ORR intermediates in a variety of aprotic electrolyte solvent candidates for $Li-O_2$ batteries. The dependence of the presence of these intermediates on ORR potential was also explored, with implications for growth mechanisms of Li_2O_2 in $Li-O_2$ cells. • A computational method to calculate the reaction energy of ion and solvent molecules has been set up, and benchmark calculations are in progress.
Industry Collaboration	• Collaborating with scientists at Liox Power (Pasadena, California) on examining solvent effects on $Li-O_2$ redox reactions.
US-China Collaboration Activities	None
Issues of Concern	None.
Notable Recent Achievements	David G. Kwabi, Betar M. Gallant, Jigang Zhou and Yang Shao-Horn, "Mechanistic studies of lithium-oxygen reactions using rotating ring disk electrode," Presented at Materials Research Society Fall Meeting; December 1 – 6, 2013; Boston, MA

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 employing combined experimental and computational approach
	• Target fuels: ortho-cymene, meta-cymene, para-cymene (potential biofuels)
	• Investigate 3 key features related to a low-temperature ignition phenomena (the *ortho*- effect) characteristic of some substituted aromatics that are relevant to diesel and gasoline applications (see list below). These results are the first of their kind, and can have significant impact on the fundamental understanding of the initial steps of substituted aromatic oxidation.
	  o Temperature-dependence of the ortho- effect in cymenes
	  o Quantification of primary low-temperature fuel consumption pathways using branching fraction measurements performed at the Advanced Light Source of Lawrence Berkeley National Laboratory
	• Determination of the effect of temperature on competing chain-propagation channels in ortho-cymene oxidation

Progress Report	• Completed: fundamental experiments on oxidation of ortho-, meta-, and para-cymene at low pressure (8 torr) and a broad temperature range (450 K – 750 K) • Purchased several high-value intermediates to directly characterize important oxidation pathways related to biofuel autoignition • Completed: calculations of all R + O_2 stationary point energies (ortho-cymene) • Planned: Laser-absorption measurements of OH, HO_2 time histories
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	• Journal publication on cymene oxidation in preparation for submission to the biannual 35th International Symposium on Combustion (August, 2014) • Initiated setup of high-pressure experimental apparatus for performing fundamental ignition-relevant fundamental chemistry measurements of low-vapor-pressure biofuels (e.g. cymenes, bisabolane). Preliminary experiments targeted for February/March 2014.

Thrust	TA 2: Advanced Biofuels, Clean Combustion and Auxiliary Power Unit (APU)
Title	**Project 1.2: Chemical and Physical Models for Novel Fuels (Cooperative US)**
Personnel	PIs: Prof. Angela Violi (UM) Graduate Student: Tyler Dillstrom (UM), Shao Teng Chong (UM)
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 explore the chemistry of fragments of said fuels and proceed to piece together their chemical kinetics from the chemistry of the various fragments. In this quarter we have continued our investigation of 2,5-dimethylhexane (a bisabolane fragment), or specifically, the low temperature oxidation of the 2,5-dimethylhexyl radical. There are 3 unique radicals of the 2,5-dimethylhexane, one primary, one secondary, and one tertiary radical. In this quarter we thoroughly explored the low temperature oxidation of the secondary radical. We developed the complete reaction pathway system, as well as the corresponding reaction rates, and the corresponding potential energy surface. We continued to input the calculated rates into the existing base mechanism for alkanes and used our modified mechanism to simulate the oxidation of 2,5-dimethylhexane in a shock tube. In this quarter we have expanded the previously studied number of low temperature pathways of 2,5-dimethylhexane. The idea is that we will be able to generate one mechanism which will be able to simulate the combustion of 2,5-dimethylhexane in wide ranges of pressure and temperature. Because several different alkyl radicals result during 2,5-dimethylhexane oxidation, there are many unique pathways we must explore. Future work will concentrate on refining the 2,5-dimethylhexane kinetic mechanism by validation with experimental data and expanding the potential energy surface of 2,5-dimethylhexane to include all the low temperature pathways.  **Figure 1.** Structures of novel biofuel molecules.

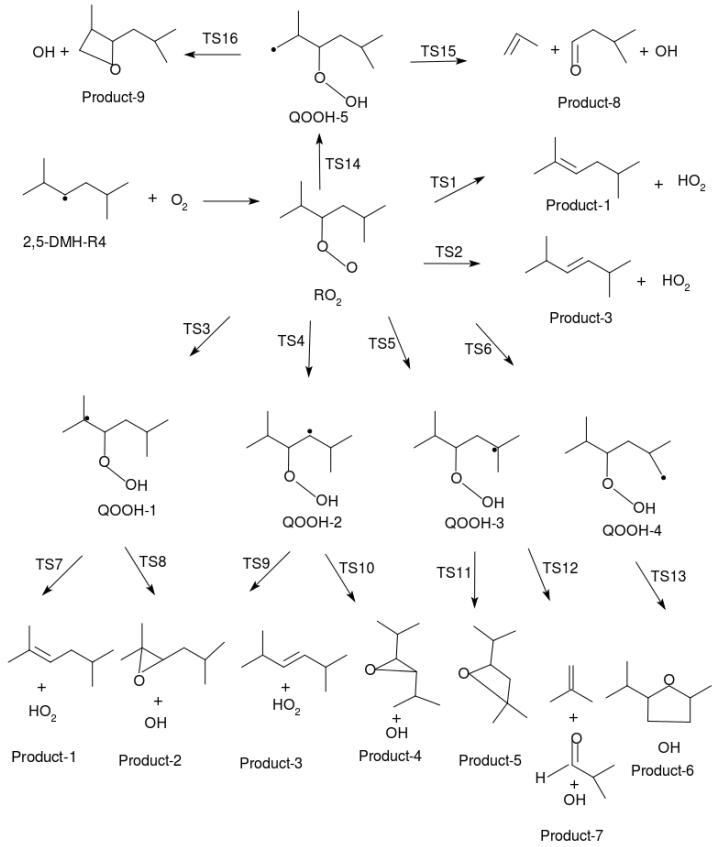


Figure 2. Reaction Pathways for the Oxidation of 2,5-Dimethylhexyl radical R2.

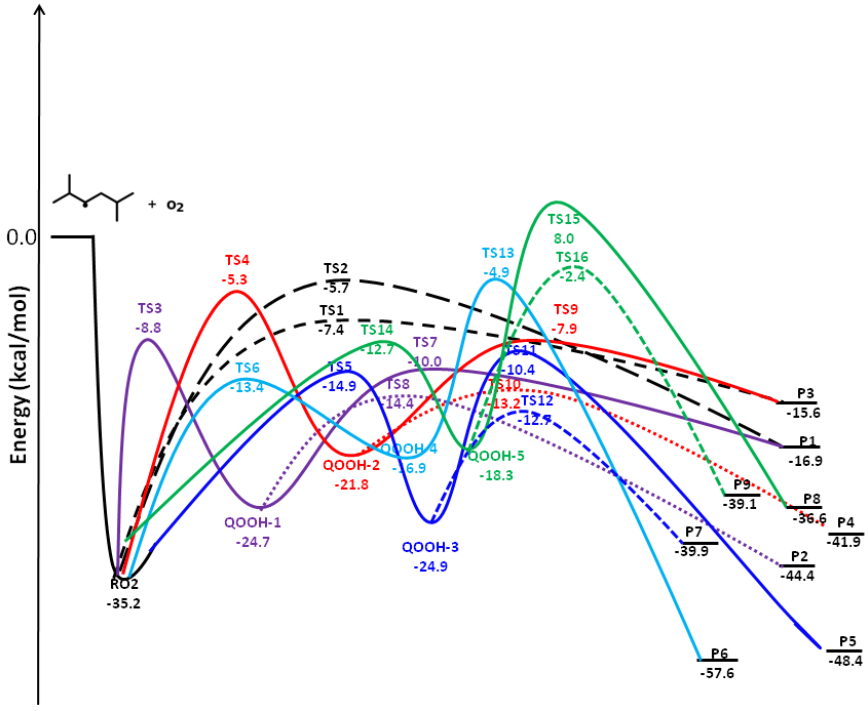


Figure 3. PES of the radical R2 of 2,5-dimethylhexane.

	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.
Industry Collaboration	N/A
US-China Collaboration Activities	Monthly Conference calls. Next month a visiting scholar from Tsinghua University will join us to collaborate on this project.
Issues of Concern	We were unable to obtain the fuel farnesane from Amyris because of legal issues. The inability to obtain farnesane requires us to change our plan for future work which involved testing the farnesane in a research engine. Now, we are in the process of trying to obtain the unsaturated farnesene and hydrogenating it to farnesane. If hydrogenating a large amount of farnesene is not possible, we will need to identify a different fuel that is suitable for all the collaborators. Update: It seems as though we will not be able to produce the amounts of farnesane necessary for our experiments from farnesene hydrogenation. We will have to focus on getting farnesane from an alternate source.
Notable Recent Achievements	**Conferences and Meetings:** (Acknowledgements to CERC-CVC) 1. Mohamad Akbar Ali and Angela Violi, Unimolecular decomposition reaction of biofuel, US-China CERC, Michigan, Ann Arbor, USA, 27-28 August, 2012. 2. Mohamad Akbar Ali and Angela Violi, Theoretical study of thermal decomposition of biodiesels fuels, 22nd International Symposium on Gas Kinetics, Boulder, Colorado, USA, 18-22 June 2012. 3. Mohamad Akbar Ali, V. Tyler Dillstrom, Jason Y. W. Lai and Angela Violi, Ab Initio Investigation of the Thermal Decomposition of n-Butylcyclohexane, 34th International Symposium on Combustion Warsaw, Poland, 29th July- 3rd August 2012. 4. Brandon Rotavera, Mohamad A. Ali, Oliver Welz, Leonid Sheps, Adam M. Scheer, John D. Savee, David L. Osborn, Taek Soon Lee, Angela Violi, Blake A. Simmons, and Craig A. Taatjes, Component-centered approach towards oxidations studies of complex biofuels. 8th International Conference on Chemical Kinetics, Spain 8th -12th July, 2013. **Research Article** 1. Reaction Pathways for the Thermal Decomposition of Methyl Butanoate Mohamad Akbar Ali and Angela Violi, *Journal of Organic Chemistry* 78(12), pp. 5898-5908 (2013) 2. Ab Initio/DFT Investigation of the Thermal Decomposition of n-Butylcyclohexane; Mohamad Akbar Ali, V. Tyler Dillstrom, Jason Y. W. Lai and Angela Violi (Accepted – Journal of Physical Chemistry A).

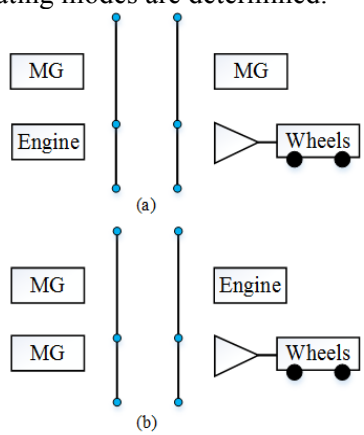
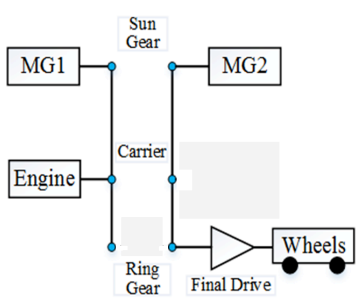
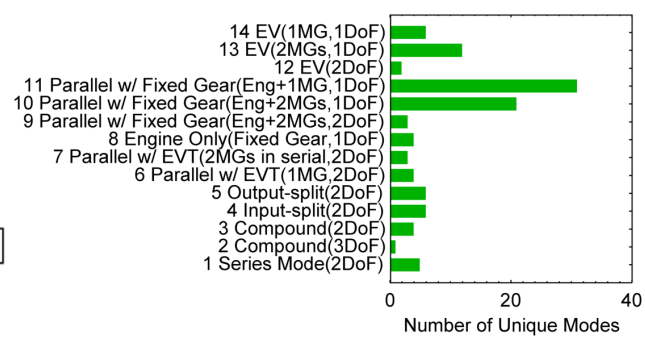
Thrust	TA 2: Advanced Biofuels, Clean Combustion and Auxiliary Power Unit (APU)
Title	**Project 2: Integrated Powertrain and Aftertreatment System Control for Clean Vehicles (Joint)**
Personnel	PI: Junmin Wang (OSU), Jing Sun (UM), Jim Parks (ORNL), Fuyuan Yang (THU), Min Xu (SJTU) Graduate students: Pingen Chen and 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 methods for simultaneous estimations of fuel blend level and intake manifold oxygen concentration. • Researched on methods for active thermal management of aftertreatment systems. • Developed observer-based air-path oxygen concentration estimation method for engines running biodiesel fuel. • Developed a combustion model applicable for Diesel and biodiesel fuels in Diesel engines.
Industry Collaboration	• We have involved CERC-CVC industry partners at 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 visited Tsinghua University again to discuss on the collaborations in July 2013 • 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 invention disclosure was filed through OSU ✓ Junfeng Zhao and Junmin Wang, "Engine onboard fuel property identification method using common rail pressure signal," Oct. 2012. The following 14 peer-reviewed papers (7 journals and 6 conferences) have been published or accepted for publication, and several other manuscripts are under review. 1. 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 (in press), 2014. 2. Pingen Chen and Junmin Wang, "Control-Oriented Model for Integrated Diesel Engine and Aftertreatment Systems Thermal Management," *Control Engineering Practice* (in press), 2013 3. Pingen Chen and Junmin Wang, "Nonlinear and Adaptive Control of NO/NO_2 Ratio for Improving Selective Catalytic Reduction System Performance," *Journal of The Franklin Institute*, Vol. 350, Issue 8, pp. 1992 – 2012, 2013 4. Pingen Chen and Junmin Wang, "Observer-based Estimation of Air-Fractions for a Diesel Engine Coupled with Aftertreatment Systems," *IEEE Transactions on Control Systems Technology* (in press), 2013 5. Junfeng Zhao and Junmin Wang, "Control-Oriented Multi-Phase

	Combustion Model for Biodiesel Fueled Engines," *Applied Energy*, Vol. 108, pp. 92 - 99, 2013. 6. Junfeng Zhao and Junmin Wang, "Effect of Exhaust Gas Recirculation on Biodiesel Blend Level Estimation in Diesel Engines," *ASME Transactions Journal of Dynamic Systems, Measurements, and Control*, Vol. 135, Issue 1, 011011, 2013. 7. Pingen Chen and Junmin Wang, "Oxygen Concentration Dynamic Model and Observer-Based Estimation through a Diesel Engine Aftertreatment System," *ASME Transactions Journal of Dynamic Systems, Measurement, and Control*, Vol. 134, Issue 3, 031008 (10 pages), 2012. 8. Pingen Chen and Junmin Wang, "Control-Oriented Modeling and Observer-based Estimation of Solid and Gas Temperatures for a Diesel Engine Aftertreatment System," *ASME Transactions Journal of Dynamic Systems, Measurement and Control*, Vol. 134, Issue 6, 061011 (12 pages), 2012. 9. Junfeng Zhao and Junmin Wang, "Observer Based Oxygen Fraction Estimation for a Dual-Loop EGR Diesel Engine Fueled with Biodiesel Blends," *Proceedings of the 2013 ASME Dynamic Systems and Control Conference* (Invited Paper), 2013. 10. Pingen Chen and Junmin Wang, "Integrated Diesel Engine and Selective Catalytic Reduction System Active NOx Control for Fuel Economy Improvement," *Proceedings of the 2013 American Control Conference*, pp. 2199 - 2204, 2013 11. Junfeng Zhao and Junmin Wang, "On-Board Fuel Property Identification Method Based on Common Rail Pressure Signal," *Proceedings of the 2012 ASME Dynamic Systems and Control Conference* (Invited Paper), pp. 2238 – 2245, 2012. 12. Junfeng Zhao and Junmin Wang, "Energy-based and Oxygen-based Biodiesel Blend Level Estimation Methods for Diesel Engines," *Proceedings of the 2012 American Control Conference* (Invited Paper), pp.4975 – 4980, 2012. 13. Pingen Chen and Junmin Wang, "Control-Oriented Modeling of Thermal Behavior for a Diesel Oxidation Catalyst," *Proceedings of the 2012 American Control Conference*, pp. 4987 – 4992, 2012. 14. Pingen Chen and Junmin Wang, "Oxygen Concentration Dynamic Model through a Diesel Engine Aftertreatment System," *Proceedings of the ASME Dynamic Systems and Control Conference* (Invited Paper), pp. 867 – 874, 2011.

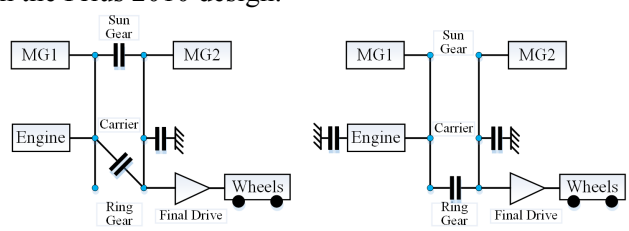
Thrust	TA 2: Advanced Biofuels, Clean Combustion and Auxiliary Power Unit (APU)
Title	**Project 4: Energy Conversion-Efficient TE Materials for Vehicle Waste Heat Recovery (Joint)**
Personnel	PIs: Prof. Ctirad Uher (UM), Prof. Rachel Goldman (UM), Prof. Kevin Pipe (UM), Prof. Joseph Heremans (OSU), Dr. Douglas Medlin (SNL), Dr. Hsin Wang, (ORNL), Prof. Xinfeng Tang (WHUT), Prof. Han Li, (WHUT) Graduate students: Si Hiu (UM), Jenna Walrath (UM), Michele Nielson (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. STM, STS, and SThEM investigations of nitric acid etched Sb_2Te_3 thin films: Both STM and STS show better tip-sample interaction compared to the non-etched one, which reveals that clean surfaces can be obtained by chemical etching. (October) 2. STM and SThEM of a bulk skutterudite polycrystalline sample: The SThEM measurement shows a large variation of the Seebeck coefficient, up to 33% from the mean, across the sample, which reveals significant inhomogeneity. (November) 3. STM, STS, and SThEM of single crystal samples of bulk p-GaAs and bulk Sb_2Te_3: Both STS and SThEM reveal uniform density of states and Seebeck coefficient across the scanned surface, with a maximum deviation from the mean of 4%. The large percent deviation of S for the skutterudite sample (33%) compared to the small value for GaAs (4%) further confirms that the SThEM technique is able to distinguish local differences between uniform single-crystal materials and non-uniform polycrystalline materials. (December)
Industry Collaboration	None, but discussions with potential industrial partner in progress.
US-China Collaboration Activities	• Prof. Uher visited the Wuhan University of Technology during December 7-15, 2013.
Issues of Concern	None
Notable Recent Achievements	**Invention Disclosure:** ✓ OSU Invention Disclosure 2013-086 was filed for "Aluminum as a resonant level in p-type CoSb3." **Publications:** • J. C. Walrath, Y. H. Lin, K. P. Pipe, and R. S. Goldman, "Quantifying the Local Seebeck coefficient using Scanning Thermoelectric Microscopy" (submitted for publication). • S. Hui, M. Nielson, D. Medlin, J. Salvador, J. P. Heremans, K. P. Pipe, and C. Uher, "Influence on the thermoelectric transport properties in $CoSb_3$-based skutterudites through incorporation of Sn" (submitted for publication). **Awards:** • R.S. Goldman elected Fellow of the American Physical Society • J.C. Walrath awarded National Science Foundation Graduate Research Fellowship

Thrust Area 3: Vehicle Electrification

Thrust	TA 3: Vehicle Electrification
Title	**Project 1: Computationally Efficient Electric Machine Design (Joint)**
Personnel	PI: Heath Hofmann (UM) Graduate Student: Jason Pries (UM)
Objective	Develop a set of computationally efficient algorithms for steady-state finite-element analysis of electric machines.
Progress Report	We are continuing our investigation into extending the harmonic balance/domain decomposition algorithm to asynchronous machines. There is an existing method for computing Fourier transforms of waveforms with two incomensurate frequencies based on a two-dimensional Fourier transform which will be used in our initial implementation. We anticipate the method will work reasonably for problems with low slip frequency. However, as the slip increases, it becomes highly desirable to have a method which allows us to compute "Fourier transforms" which include arbitrary combinations of two fundamental frequencies, along with a way to adaptively select those frequencies. We are continuing efforts to import our models into commerical software in order to validate our code. 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.
US-China Collaboration Activities	• Starting February 1st, we will be hosting a Tsinghua student, Ziyou Song, who will be working in our research laboratory for one year..
Issues of Concern	• No appreciable issues of concern at this time.
Notable Recent Achievements	We have developed a preconditioner which significantly reduces the computation time of our steady-state solver. More importantly, the computation time scales almost linearly with the size of the problem, allowing the solver to be used on problems with high fidelity.

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. 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)
Objective	The objective of this project is to develop vehicle models, design and control tools for the system integration, diagnosis of electric powertrains, and NVH performance analysis. The ultimate goal is to enable rapid powertrain designs and integration that improve the reliability and achieve optimal efficiency for clean vehicles.
Progress Report	• Over the last quarter, we continued to develop a systematic design procedure for hybrid vehicles with two planetary gears and multiple clutches. The procedure includes three parts: Automated modeling, mode screening and mode classification. • In previous reports, we confirmed that for double planetary gear system, with 2 electric machines (motor/generator) and 1 engine as powertrain components, there are 360 different configurations. In addition, for each configuration, in theory a total of 21 clutches could be installed. In-depth analysis shows that we only need to analyze 216 configurations each with up to 16 clutches after infeasible and redundant designs were eliminated. Topologically, the configurations can be categorized into 2 different types, as shown in the figure below, depending on whether the engine and vehicle are located on the same planetary gear or not. Once the type of configuration is fixed, the number and characteristic of the operating modes are determined.  • As a case study, one type (a) of configuration (#83), which is also the configuration of Prius (MY2010), Camry and Highlander Hybrid has been chosen. There are a total of 109 possible modes, and they were grouped into 14 different categories and are shown below. Even though we know there are many modes possible, it is apparent it is neither necessary nor beneficial to use all 109 modes.  Configuration #83 

- We combined PEARS – the previously developed fast optimization method, together with this automatic modeling and mode identification approach to find the optimal clutch location for configuration #83. For practical reasons, we constrained the clutch number to be 3, which is the number of clutches deployed on GM Volt, which we assume reflects the level of complexity and cost that is bearable on production hybrid vehicles. This 3 clutch configuration give us C_{16}^{3} different location combinations. For each of the 3-clutch sub-optimal designs, we solve the optimal mode selection and power split control problem using PEARS. The optimization results show that for the city cycle, 25 HEV and 18 PHEV designs achieve better fuel economy than Prius2010 (when the same engine/motors are used). If both city and highway performance are considered—i.e., the fuel consumption of the city/highway cycles are combined 55/45, even more designs achieve better fuel economy: 50 for HEV and 39 for PHEV. Two examples designs are shown below. These are not the configurations that achieve the best fuel economy—the best are being analyzed more closely for possible patent applications. The configuration (a) shown below uses primarily parallel modes and configuration (b) shown below can be said to be "Prius++", i.e., similar to the Prius MY 2010 design, except that three clutches are added to enable extra modes. Both configurations achieve roughly 7% better fuel economy compared with the Prius 2010 design.



- Besides achieving better fuel economy, multiple-clutch designs can also deliver good drivability. The launching power available for the two configuration examples above are shown in the Figure below. The launching performance and the fuel economy of the two configurations are summarized in the table below.
- The take away lesson is that if we exhaustively search through all possible configurations and operating modes, much better drivability and fuel economy is possible, even when exactly the same engine/motor/generator are used. Whether the additional cost and complexity associated with the added clutches is worthwhile or not is a question that we aim to answer by closely consulting our industrial members.

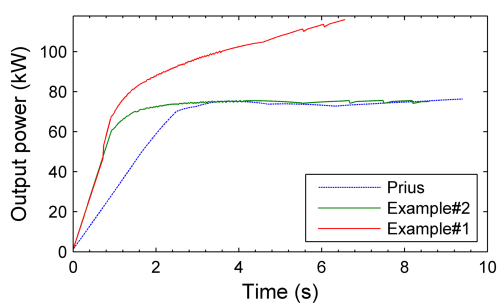


TABLE COMPARISON BETWEEN PRIUS AND EXAMPLE PHEV DESIGNS

Designs	Example #1	Example #2	Prius
0 to 60mph(s)	6.6	8.6	9.5
Normalized fuel consumption	92.8%	93.3%	100%

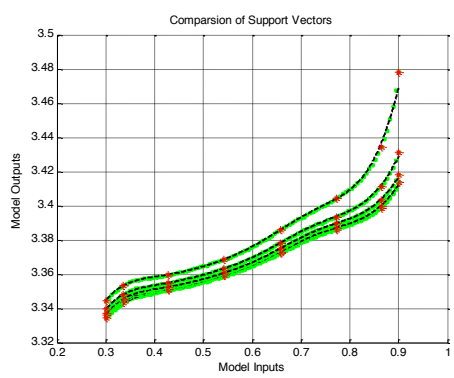
Industry

- The 1PG results have been shared in our TA project review meeting to all CERC

Collaboration	industrial members. We had held meetings to seek input from Ford HEV expert Ming Kuang (Ford Research). A meeting with the production group (Powertrain Product Development) is now being scheduled working with Daniel Kok.
US-China Collaboration Activities	• We have presented in our monthly technical meetings in November 2013.
Issues of Concern	N/A
Notable Recent Achievements	• Xiaowu Zhang, Huei Peng, Jing Sun, "A Near-Optimal Power Management Strategy for Rapid Component Sizing of Power Split Hybrid Vehicles with Multiple Operating Modes", 2013 American Control Conference, Washington DC.

Thrust	TA3: Vehicle Electrification
Title	**Project 3.2 Intelligent Fault Diagnosis and Prognosis (Joint)**
Personnel	PI: Giorgio Rizzoni(OSU), Dr. Hongmei Li (HFUT) Post Doc Researcher: Dr. Qadeer Ahmed (OSU) Graduate Students: Jiyu Zhang (OSU), Andrea Cordoba Arenas(OSU) Visiting Scholar: Assoc. Prof. Qi Chen (HFUT), Zhentong Liu, PhD Student (BIT)
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	• A diagnostic strategy based on conventional Luenberger observers has been developed for PMSM drive system in HEV/EV, with focus on sensor faults. The strategy can work well when the vehicle is in cruise control (constant speed region). We utilized two generalized observers to detect and isolate current sensor, speed sensor as well as position sensor faults that are common to PMSM drive system. (Jiyu Zhang) • We have done structural analysis for PMSM drive system using graphical tools (bipartite graphs and directed graphs) for fault detectability and isolability analysis. In the future, we plan to develop FDI strategies and tools for PMSM drive system in HEV/EVs based on structural analysis. (Jiyu Zhang) • We have conducted a hazard analysis for Lithium-ion battery systems through fault tree analysis (FTA) and failure modes and effect analysis (FMEA) from chemical, electrical and mechanical perspectives. In the next step, we plan to develop a FDI strategies for battery systems based on structural analysis from cell level to pack level, with special focus on sensor faults, i.e. current, voltage and temperature sensors faults. (Zhengtong Liu)
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 August 2013. • 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] Cordoba-Arenas, A., Onori, S., Giorgio, G., Fan, G. Aging Propagation in Interconnected Systems with an Application to Advanced Automotive Battery Packs. *2013 IFAC Symposium Advances in Automotive Control,* Japan, September, 2013 [2] Cordoba-Arenas, A., Zhang, J., Giorgio, R., Diagnostics and Prognostics Needs and Requirements for Electrified Vehicles Powertrains. *2013 IFAC Symposium Advances in Automotive Control,* September, 2013 [3] Zhang, J., Giorgio, R., Ahmed, Q., Fault Modeling for Hierarchical Fault Diagnosis and Prognosis. *2013 ASME Dynamic Systems and Control Conference Automotive and Transportation Systems*, October 21-23

Thrust	TA3: Vehicle Electrification
Title	**Project 4.1: Adaptive battery management system on and off the grid (Joint)**
Personnel	PIs: Prof. Jing Sun (UM), Prof. 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 fourth quarter of 2013, 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. A parametric battery model could be developed from single cell data and applied to other cells in the same pack. Comparing to applying SVR to each 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 fourth quarter of 2013 have been focused on (a) investigation on how the locations of support vectors change for the SVR model when a battery ages; (b) Establishing a support vector based parametric model and verifying the model robustness for battery data at all ages. (c) Exploring the model structure from both physical and mathematical perspectives. For parts (a) and (b), we applied our SVR algorithm to all battery aging data and let the optimization algorithm decide where the support vectors should locate. Aging data of both LiFePO4 and LiNMC batteries are used in this study. For LiFePO4 cells, the support vectors do not change their positions as the battery ages. For LiNMC, the support vectors are also fixed after initial break-in periods. Therefore, a parametric model may be built based on the SVR model and the parameters can be identified using the least squares methods instead of an iterative optimization algorithm. 

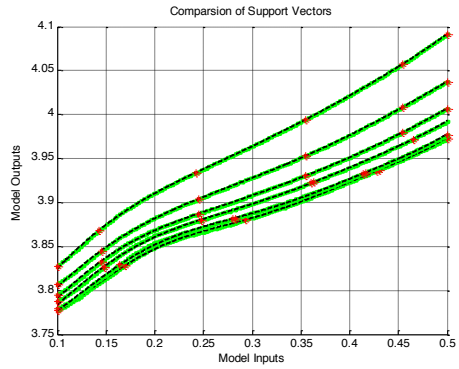


Figure 1: Positions of support vectors on battery charging curves at different ages

The invariant properties of the support vectors have been explored in two different directions. From the physical perspective, we are attempting at associating the positions of the support vectors with lithium ion intercalation process and gaining insights on how this connection can be used to explain and characterize battery aging mechanisms. On the other hand, we are also investigating the implications of the invariant support vectors on the linear programming algorithms, in order to generalize the support vector based parametrization methods.

In parallel, we are continuing the battery aging data collection on the Abion test bench. Two dynamic discharging profiles that emulate urban and suburban (using UDDS and HWY drive cycles from EPA) driving conditions respectively, are being used. Initial results show that the urban driving cycle ages the battery cells faster.

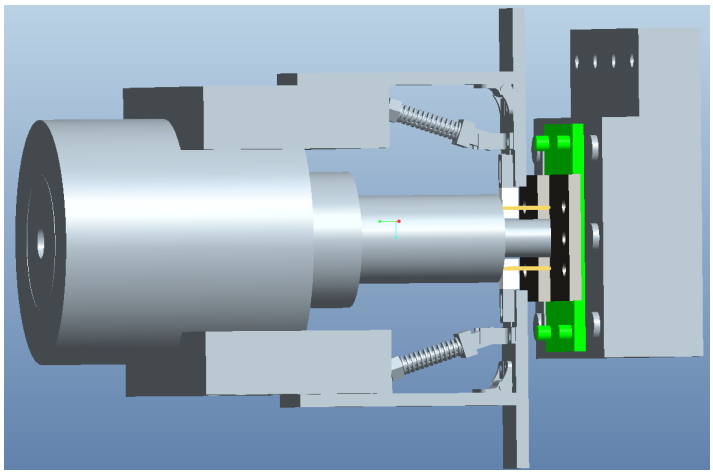
In the next quarter, the team will continue to focus on the development of adaptive battery management system. Efforts will be directed to establishing real-time individual cell degradation detection using SVR based model parametrization. A "virtual" battery pack simulation will be used and cell-to-cell variance will be considered. The physical properties of lithium intercalation process will be further explored.

Industry Collaboration	None
US-China Collaboration Activities	• The visiting plan of a Tsinghua student is being finalized
Issues of Concern	None
Notable Recent Achievements	A paper on OCV model for SOC and SOH estimation was presented at ASME DSCC 2013

Thrust	TA 3: Vehicle Electrification
Title	**Project 4.2: Data-Based Techniques for Battery-Health Prediction (US Cooperative)**
Personnel	PIs: Dennis S. Bernstein (UM), Jeffrey L. Stein (UM) Research Scientist: Tulga Ersal (UM) Graduate student: 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	• Side reaction current density, the electrochemical feature that directly relates to capacity fade, was proposed as our new metric for battery degradation. By estimation the side reaction current density, we are able to track the capacity fade of the battery over time. This new degradation metric can be used to track the battery degradation caused by all electrochemical-based mechanisms. • Reconstructed the battery model for estimation of side reaction current density. • Developed the linear version of the battery model based on the reconstruction. • Applied RCMR to the linearized battery model. The estimated subsystem parameter and output are accurate to a certain level. Sensitivity to both measurement noise and the impact of initialization error are tested.
Industry Collaboration	• None
US-China Collaboration Activities	• None
Issues of Concern	• None
Notable Recent Achievements	• Best Student Paper Finalist: X. Zhou, T. Ersal, J. L. Stein, and D. S. Bernstein, "Battery health diagnostics using retrospective-cost system identification: Sensitivity to noise and initialization errors," Dynamic Systems and Control Conference, Palo Alto, CA, 2013.

Thrust	TA 4: Advanced Lightweight Materials and Structures
Title	**Project 2: Cost Effective Light Weight Materials (Cooperative US)**
Personnel	PIs: Prof. Glenn S. Daehn, Prof. Jose Castro (OSU) Graduate Student: Ziwei Zhao (OSU)
Objective	To develop cost-effective light weight structures for next generation vehicle. A key barrier is the balance of processability and performance of the new composites. Our project focuses on developing nano-enhanced Fiber reinforced Polymeric Composites (FRPCs) with adequate processability. One method to do so is to put a CNF nanopaper or spray nanoparticles on the surface of glass fiber in the composites.
Progress Report	In the past three months, a series of experiments that compare the flexural strength of samples with different amount of nanoparticles have been performed. Both glass fiber and carbon fiber were used to fabricate composite samples. For carbon fiber composite, the addition of nanoparticles will make the sample last longer during the experiment. For glass fiber composite, 1.2 wt% of nanoparticles will make the sample even worse; however, 2.1 wt% of nanoparticles will make the sample last longer during the experiment.
Industry Collaboration	Nano Materials Innovation, a spinoff company from OSU, collaborates in the surface modification of nanoparticles.
US-China Collaboration Activities	One journal paper was published jointly. • Zhao, Ziwei, Na Zhang, Yunior Hoie, L. James Lee, and Jose M. Castro. "Properties and process ability of long fiber-reinforced polymeric composites." Polymer Composites (2013).
Issues of Concern	• Currently, nanoparticles were demonstrated to be useful to enhance the flexural performance of polymer composites. However, the optimized amount of nanoparticles needed still needs more effort to be investigated.
Notable Recent Achievements	• Zhao, Ziwei, Na Zhang, Yunior Hoie, L. James Lee, and Jose M. Castro. "Properties and process ability of long fiber-reinforced polymeric composites." Polymer Composites (2013).

Thrust	TA 4: Advanced Lightweight Materials and Structures
Title	**Project 3.2: Conformal Interference Joining (Cooperative US)**
Personnel	Prof: Glenn S. Daehn(OSU), Anthony Luscher (OSU) Graduate Students: Steven Hansen, (OSU)
Objective	• The objective of the project has been to develop new methods of joining dissimilar metals in vehicle structures. The initial work was based on conformal interference joints, the development of which technology we believe is ready for transition into specific geometries. Technology Readiness Level 3 has been achieved, and TRL 5 could be rapidly achieved. • More 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. • The current objective is to understand and characterize the vaporizing foil launch process that can accelerate sheet metal to over 1 km/s within a few mm for collision welding.
Progress Report	• Previously performed experiments systematically varied foil thickness and input energy to characterize the relationship between energy deposition into the foil and the spacial/temporal evolution of the flyer velocity – and therefore, indirectly, the effect on the pressure development from the vaporizing foil. • The mechanical efficiency of the process depends on plasma confinement, and the strength of the flyer material effects confinement. Therefore, similar experiments are now underway which vary the flyer material and thickness in addition to the foil thickness and input energy, in order to develop an understanding of how the pressure development and resulting flyer velocity are affected. Velocity (using photonic Doppler velocimetry), voltage, and current histories are recorded for all experiments. This work was delayed in December while waiting for experiment components to be machined. • Sample assemblies with two welds in series between the same two sheets were created, in an effort to create an aluminum-steel part containing multiple joints.
Industry Collaboration	None
US-China Collaboration Activities	Nothing significant this period.
Issues of Concern	None
Notable Recent Achievements	**Submitted Publications:** • "Vaporizing Foil Actuator: Controlling the Pressure Pulse for Impulse Metalwroking", S. R. Hansen, A. Vivek and G. S. Daehn, Submitted to Proceedings of the 2014 ASME Manufacturing Science and Engineering Conference, June 9-13, 2014, University of Michigan, USA. • "High Strain Rate Metalworking with Vaporizing Foil Actuator: Control of Flyer Velocity by Varying Input Energy and Foil Thickness"", A. Vivek, S. R. Hansen and G. S. Daehn, Submitted to *Review of Scientific Instruments,* September 2013 **Publication:** • "Vaporizing Foil Actuators: A Tool for Collision Welding", A. Vivek, S. R. Hansen, B. C. Liu, G. S. Daehn, *Journal Materials Process Technology,* **213**, pp. 2304-2311 (2013).

Thrust	TA 4: Advanced Lightweight Materials and Structures
Title	**Project 3.3: Friction Stir Welding of Dissimilar Metals (Joint)**
Personnel	PIs: Prof. Jun Ni (UM), Xinmin Lai (SJTU) Post Doc: Shuhuai Lan (UM) Graduate Students: Xun Liu (UM)
Objective	Develop high-quality and economical joining processes between dissimilar lightweight materials.
Progress Report	An experimental setup has been designed, manufactured and tested for the hybrid Friction Stir Welding (FSW) process incorporating electroplastic effect. The overall CAD design is shown in Fig.1.  Fig.1 CAD design for the hybrid Friction Stir Welding system to introduce high density current In order for the electrodes to move along with the FSW tool and therefore ensure the electrical current field remains surrounding the weld zone, two aluminum blocks were fabricated to clamp onto the shell of the CNC spindle. Electrodes were made of copper and mounted to these two aluminum blocks through fixtures shown above. Two pieces of perpendicularly positioned aluminum board were connected through a hinge with a compressive spring supporting in between. The force exerted by the spring can be adjusted to achieve a close contact between electrodes and workpiece. An adjustment device with three degrees of freedom was attached at the free end of the vertical aluminum board to modify the location of electrode on the workpiece. Fig.2 and Fig.3 show a locally zoomed-in view for the electrode and workpiece configuration. The electrode was bent into curved shape to obtain a small contact area with the workpiece, which can help increase current density on the workpiece under same amount of total current. An electrically insulated coating was applied at the outer region of the electrode, which serves to eliminate undesired contact and the resulting arc generation when translating electrodes along the workpiece. Mica blocks were inserted between electrode and adjustment device to guarantee electrical insulation for the shell of the CNC spindle. Since steel possesses a much higher deformation resistance than aluminum, both of the electrodes were positioned in the steel side for the current consideration. Electrical insulation coating was applied in the chuck for clamping the FSW tool into spindle without introducing current into the spindle. Insulation between workpiece and backing plate was accomplished through a sheet of mica based on its favorable insulation properties under high temperature.

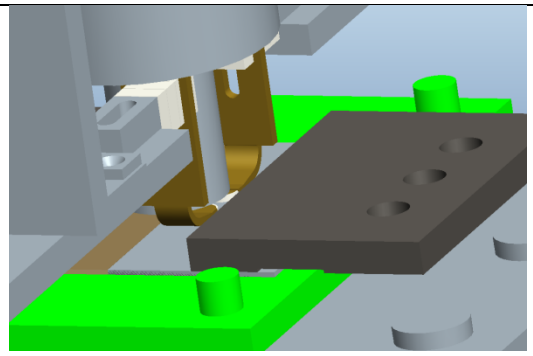


Fig.2 A locally zoomed-in view for electrodes and workpiece configuration

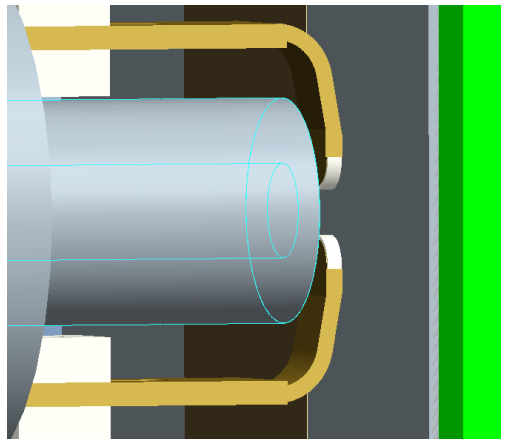


Fig.3 A locally zoomed-in view for the shape of electrodes

Fig. 4 shows the actually manufactured fixture and Fig. 5 shows the whole setup on ground for insulation test. A more detailed top down view and zoomed in view are given in Fig. 6 and Fig. 7.

Fig. 4 The actually manufactured fixture for connecting aluminum block and electrode

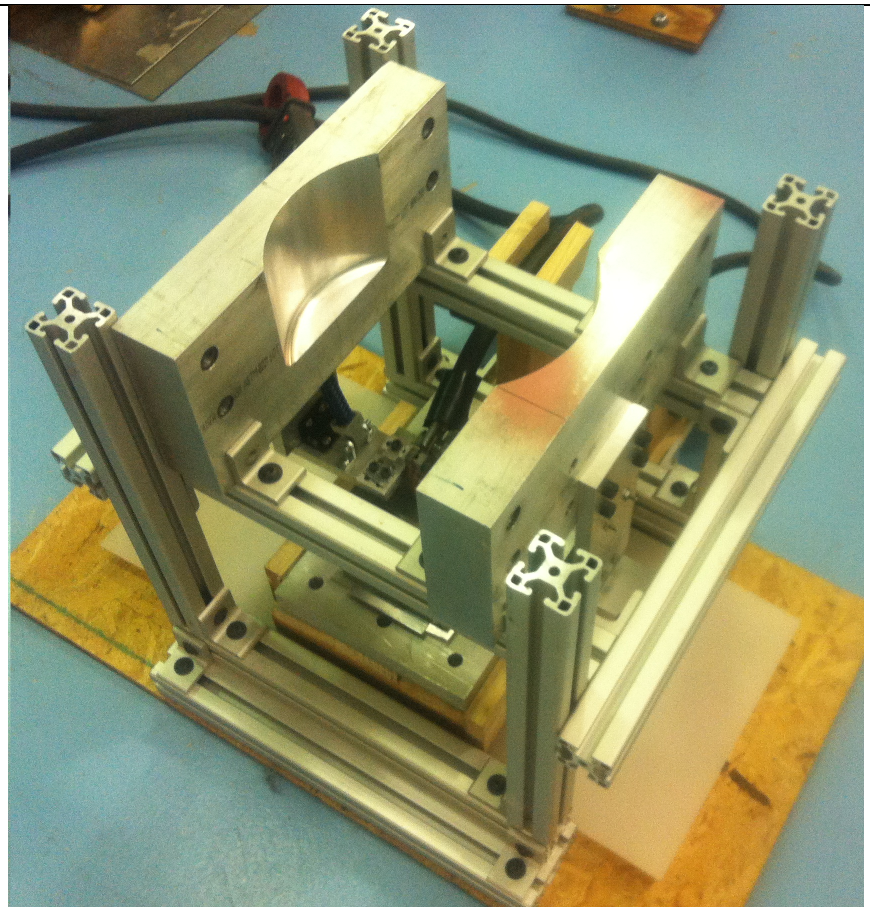


Fig. 5 Overview of the whole setup for introducing high current into FSW process and the setup was placed on ground for insulation testing

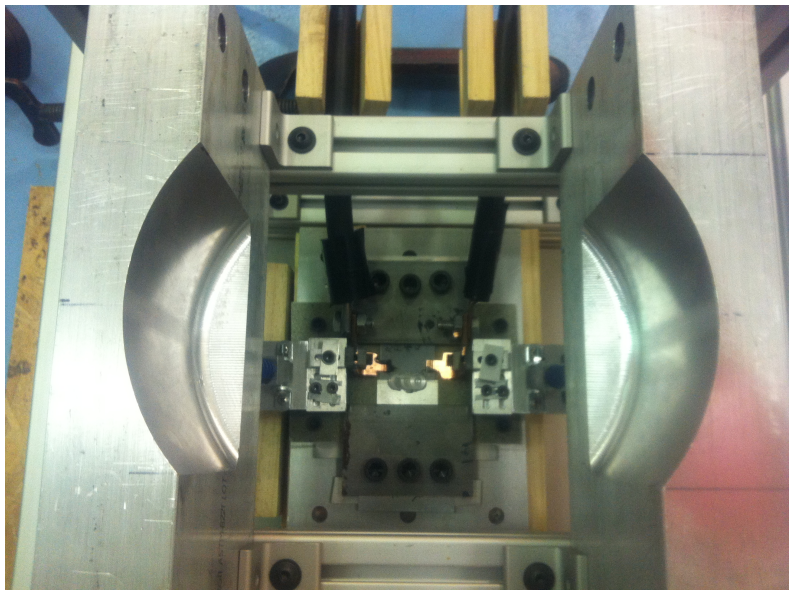
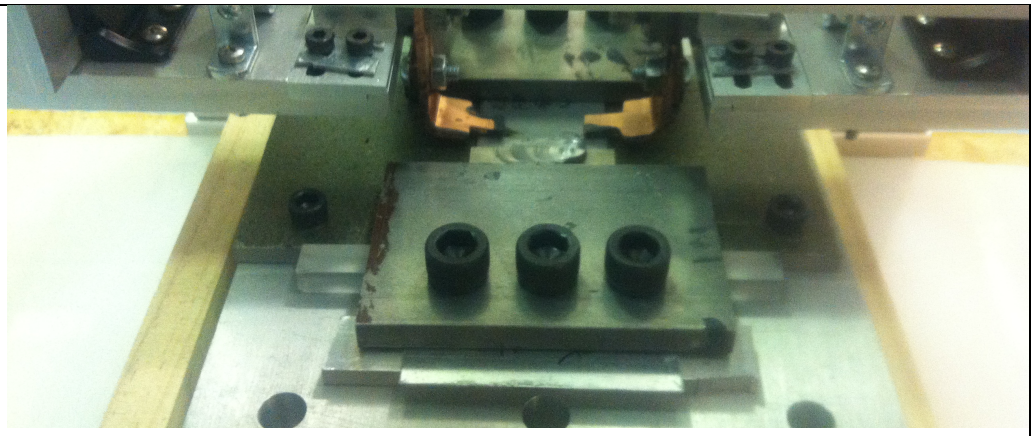
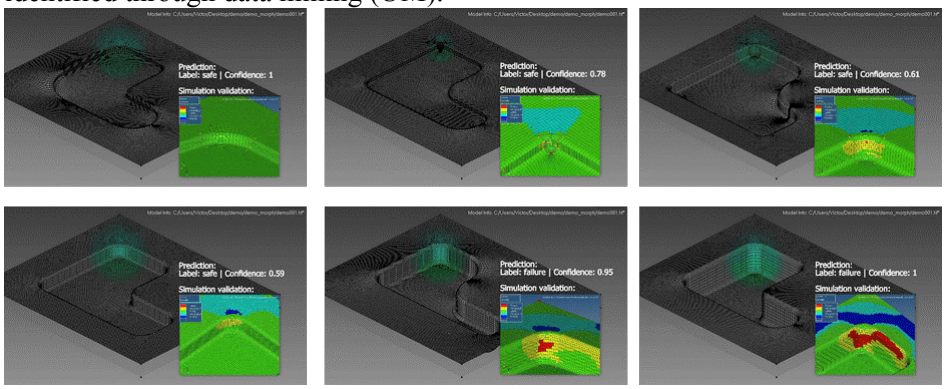
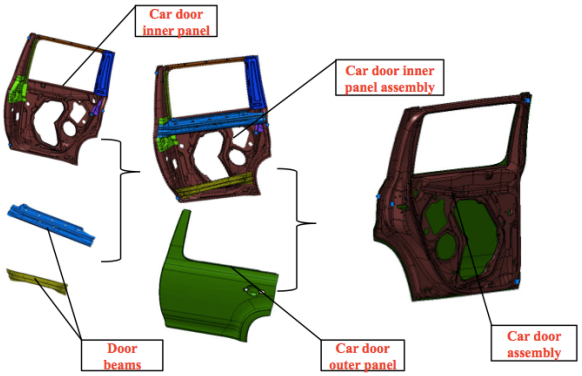


Fig. 6 Top down view of the setup

	 Fig. 7 Zoomed-in view of the setup Electrical insulation for the aluminum blocks and backing plate has been tested. It was shown to be acceptable for a moving workpiece with regard to electrodes when a total current of 260A was applied. In addition, one second pulse of 260A current did not cause significant heating on the workpiece. Further tests will be performed for the hybrid FSW process. A finite element model has also been established in Abaqus to simulate the plunge stage of FSW for different materials. Convergence was difficult to achieve due to the extreme element distortion as well as the unstable contact between aluminum and steel. Three strategies have been adopted for handling this problem: Arbitrary Lagrangian-Eulerian (ALE) mesh, adaptive remesh and element progressive damage and failure. Computational cost for ALE is too high and failure of element generated a large hole in the workpiece. Combination of these two methods are being taken into consideration.
Industry Collaboration	N/A
US-China Collaboration Activities	N/A
Issues of Concern	• Sparks generated when translating the workpiece against electrodes under a total current of more than 300A.
Notable Recent Achievements	Invention Disclosure: ✓ UM Invention Disclosure #5675 was filed for "Hybrid Friction Stir Welding for dissimilar materials through Electro-Plastic Effect." Publications: • X. Liu, S. Lan, J. Ni "Friction stir welding of dissimilar aluminum alloys to advanced high strength steel," Journal of Materials Processing Technology (under review) • X. Liu, S. Lan, J. Ni "Comprehensive analysis on the effects of process parameters on friction stir welding of dissimilar aluminum alloy to advanced high strength steel," Materials & Design (submitted)

Thrust	TA4: Advanced Lightweight Materials and Structures
Title	**Project 3.4: Hybrid Materials Interface Increase Strength Method and Modeling (Cooperative US)**
Personnel	PIs: M.D. Thouless (UM) Graduate student: 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 in objective
Progress Report	• The GSRA has made some DCB specimens to obtain experience in bonding them, and has done some initial tests. The GSRA has also started getting experience with the numerical code. • However, this was done for mode-I geometries. A meeting with the industrial partner identified the fact that mode-II dominated bonds were of more direct interest. This required a re-focus of the approach, and a new strategy to be more industrially relevant. • The concept for how the experiments might be performed and how to analyze them results has now been established. Ongoing work is needed to validate this approach and to optimize the analysis techniques. • A paper on the physics of cohesive zones has been submitted for publication by the PI. Ongoing collaboration with a Danish colleague has identified some techniques by which experimental data might be obtained.
Industry Collaboration	• Regular conference calls with Eaton • Site visit by Peter Fritz to UM on December 11, 2013 to discuss strategies.
US-China Collaboration Activities	N/A
Issues of Concern	None
Notable Recent Achievements	N/A

Thrust	TA4: 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 (TSU), Xinmin Lai (SJTU), Zhigang Yang (Tongji) Faculty participants: Liang Tang (THU), Yongbing Li (SJTU) Graduate student: Yuqing Zhoou (UM), Zhongqi Yu (SJTU), Hua Wang (SJTU)
Objective	Develop a methodology for economically integrating components made of lightweight materials (Al, Mg, HSS/UHSS) in a vehicle body structure with maximum weight reduction benefit
Progress Report	• Empirically confirmed 1) stamping failures (i.e., wrinkling and tearing) mostly occur at certain local geometric features (eg., deep drawn corner), 2) occurrence of failure is affected by a small number of parameters that specify the geometry of local features (eg., corner radius and draw depth), mostly independent of the overall part geometry (UM) • Successfully demonstrated the data-mined design guidelines outperforms well-established design guidelines found in a SME handbook (UM) in terms of the binary (i.e., black and white) prediction accuracy of stamping failures in parts with various geometry (UM). • Developed an algorithm to compute confidence values of the design guidelines identified through data mining (UM).  • Simulated the deformation of a car door after installation due to the temperature variation caused by daily use or low-temperature baking, and the impact of CFRP/Al composite structure of the bumper beam on the deformation (SJTU).  • Studied how mass distribution of battery and occupants would influence crash response in mini-EV. Battery layout influences crash pulse through CG location and pitch effect, and vehicle pitch affects crash energy absorption. The number of occupants affects crash pulse through CG location and added weight (THU-Zhou). • Demonstrated the use of HSS in mini-EV frame does not have significant effect on weight reduction as the mass of the frame is only about 20% of the total weight (THU-Zhou)
Industry Collaboration	FEV, Inc, a contractor of EPA/Venza project, provided us with the scanned CAD model for Toyota Venza, which is used to benchmark the design guidelines obtained by data mining.

US-China Collaboration Activities	Continued to interact with SJTU team to compile DFM constraints for HSS/UHSS stamping based on the ones for conventional mild steel.
Issues of Concern	• While Tsinghua team agreed to give us the CAD model of mini- or micro-EV (year 5 demo platform), its delivery is delayed (UM)
Notable Recent Achievements	• Wrote a draft paper titled "Identification of Manufacturability Constraints through Process Simulation and Data Mining" to be submitted to ASME Design for Manufacturing and the Life Cycle conference to be held in August 2014.

Thrust Area 5: Vehicle Grid Integration

Thrust	TA 5: Vehicle Grid Integration
Title	**Project 2: Vehicle-Grid System Modeling for Technology Deployment (Joint)**
Personnel	PI: Ramteen Sioshansi (OSU), Ian Hiskens (UM), Songbin Sun (THU) Graduate Student: Fei Wu (OSU), Xiaoli Liu (OSU), Chiara Fiori (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	• Further development of pricing schemes and models to coordinate PEV charging with power system dispatch and operations and wind availability • Supplemental work on price-based PEV charging coordination, in response to referee reports on manuscript submitted for publication • Modeling cases with random PEV arrival and departure times, multiple load aggregators, and wind uncertainty to determine effectiveness of our proposed price-based charging control under these scenarios, which differ from the stylized case assumed in our theoretical results • Beginning econometric modeling to study spatial effects on alternative vehicle adoption • Collected vehicle registration data for entire state of Ohio • Used geographical information system software to match vehicle registration data to U.S. Census Blocks • Collected demographic and socio-economic data for U.S. Census Blocks and Tracts • Beginning work examining distribution transformer-effects of level-3 fast charging stations
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 and FirstEnergy have expressed interest in also examining optimization of deployment of level-3 charging infrastructure, which would build off of work done examining levels-1 and -2 charging • 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	• Ramteen Sioshansi has been invited as a keynote speaker at the 2013 IET Renewable Power Generation conference in Beijing, China • Ramteen Sioshansi has been invited as a keynote speaker at the 2013 APEC-sponsored conference on smart grid in Suzhou, Jiangsu, China • 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," revised and resubmitted for review to *IEEE Transactions on Smart Grid*.

Thrust	Thrust 5: Vehicle-Grid Integration
Title	**Project 3: Control strategies for vehicle-grid integration (Joint)**
Personnel	PIs: Ian Hiskens (UM), Hongbin Sun (THU), Qinglai Guo (THU) Student: 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	• Simulated a realistic distribution power system using three phase power flow solution algorithm to analyze voltage dynamics and effects on transformers. • Added coordinated electric vehicle loads under additive-increase multiplicative-decrease (AIMD) distributed control to assess the impact that large, variable power profiles have on power quality. • Currently quantifying the oscillatory behavior of radial networks under certain AIMD control paradigms, and working to eliminate these effects using aperiodic duty cycles.
Industry Collaboration	
US-China Collaboration Activities	• Participated in web-based meetings with US and Chinese collaborators. • Recently gave a presentation of the past year's work at the annual CERC-CRV Beijing conference, as well as getting a more in depth understanding of ongoing work of our colleagues at Tsinghua University, Beijing Institute of Technology, and Ohio State.
Issues of Concern	None
Notable Recent Achievements	Completed internship at Los Alamos National Lab involving power system demand response scenarios, with applications to current work on electric vehicle control

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

Thrust	TA6: Energy Systems Analysis, Technology Roadmaps and Policy
Title	**Project 1: Vehicle Design and Assessment (Joint)**
Personnel	PI: Gregory Keoleian (UM), Jarod Kelly (UM) Research Scientist: Jarod Kelly (UM) Graduate Student: Mohammad (Arman) Golrokhian (UM) Collaborator – Lingjun Song (Beihang University)
Objective	• Our Visiting Scholar is conducting life cycle assessment analysis of wireless charging • Evaluate the effect of recycling allocation methods on magnitude and timing of GHG emissions in vehicles' life cycle • Compare Recycled-Content (RC) and End-of-life-Recycling (EOLR) allocation methods in a fleet scenario based vehicle production. (The case study is hood of a car, however results are transferable and can be easily modified for other components) • Calculate payback periods. How long will it take for added energy and GHG in production phase to be paid back in vehicle operation phase? (Both for individual and fleet scenario) • Analyze primary and secondary mass reduction effect on payback periods
Progress Report	October 2013 • Developed the research topic, in order to find the potentials for mass reduction in vehicles and evaluate the importance of allocation methods. November 2013 • Conducted the literature review for generating scenario parameters. Most realistic scenarios developed and modeled. December 2013 • Developed the framework for comparing RC and EOLR allocation methods with different scenarios of interest. • The effect of recycling at hood's end of life is going to be studied in the next phase.
Industry Collaboration	October 2013 • Developed the research topic, in order to find the potentials for mass reduction in vehicles and evaluate the importance of allocation methods. November 2013 • Conducted the literature review for generating scenario parameters. Most realistic scenarios developed and modeled. December 2013 • Developed the framework for comparing RC and EOLR allocation methods with different scenarios of interest. • The effect of recycling at hood's end of life is going to be studied in the next phase.
US-China Collaboration Activities	• Continued thrust area meetings with industry partners • Presented annual review to industry partners
Issues of Concern	• Met with Prof. Chris Mi of UM-Dearborn to discuss the potential of conducting LCA on wireless charging system via visiting Chinese scholar
Notable Recent Achievements	• Dr. Kelly will be leaving UM for Argonne National Labs

Thrust	TA6: Energy Systems Analysis
Title	**Project 2.1: Parametric Analysis of Biofuels in the Light Duty Fleet (US Cooperative)**
Personnel	PIs: Dawn Manley (SNL), Todd West (SNL), Garrett Barter (SNL), Jessica Westbrook (SNL)
Objective	Parametric analysis of biofuels production and use in the light duty fleet
Progress Report	• Parametric analysis of the feasibility of and opportunities for large-scale penetration of clean vehicle and fuel technologies in the light duty transportation sector.
Industry Collaboration	• Completed parametric analysis of technology advancement and policy tradeoffs as they pertain to the biofuels requirements of the Renewable Fuels Standard (RFS2) in the US light-duty vehicle fleet from today through 2022 and beyond. Manuscript accepted and published in *Energy Policy*. Our results identified the key barrier to the light duty fleet using more biofuel is the fuel price differential with gasoline and not refueling station availability. The economic conditions that could lead to RFS2 compliance in the short term might discourage use of biofuels in the long term as other alternative vehicles that do not use any sort of gasoline blendstock will be attractive. • Incorporated model enhancements that account for real world driving behavior based on industry input. • Expanding scope of questions on technology & policy issues that can be addressed with the model. Implementing different models of consumer interpretation of range & public charging limitations and their influence on EV adoption.
US-China Collaboration Activities	• Discussed model approach and input data with industry partners.
Issues of Concern	• None
Notable Recent Achievements	• None

Thrust	TA6: Energy Systems Analysis
Title	**Project 2.2: Fuel mix strategies and constraints (Cooperative US)**
Personnel	PI: Ming Xu, (UM) Graduate Student: Hua Cai, (UM), Tricia Pontau (UM); Yi Zhen (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 5.
Progress Report	October: Continue collaboration with Sandia National Lab to evaluate fleet level water consumption based on their fleet model. Attended UM Energy Institute Symposium to present land and water impact of clean vehicle systems and won second place poster award. November: Conducted sensitivity analysis for land impact of clean vehicles. Assessed land constraints on production capacity of transportation fuels produced from wind, solar, and biofuel sources at the state level. December: Drafted paper titled “Assessing Land Use Impact by Clean Vehicle Systems” based on the research.
Industry Collaboration	In contact with Microsoft Research Asia for potential collaborations
US-China Collaboration Activities	Attended TA6 CERC Web-Ex Meetings
Issues of Concern	None to date
Notable Recent Achievements	• Poster titled "Resource Implications for Clean Vehicle Systems" won second place award at UM Energy Institute Symposium. • Manuscript titled “Assessing Land Use Impact by Clean Vehicle Systems” in preparation.

Thrust	TA6: Energy Systems Analysis, Technology Roadmaps and Policy
Title	**Project 4.1: Fleet modeling on China's in-use vehicle fleet (Cooperative US)**
Personnel	PI– Prof. John Heywood (MIT) Graduate Student –Summer Zhao (MIT)
Objective	• Compare the results of future vehicle stock, fuel consumptions, and CO2 emissions from models including FLEET (MIT), EPPA (Emissions Prediction and Policy Analysis, MIT), and TCAEM (Tsinghua China Automotive Energy Model). • Find out the underlying assumptions and reasons for the difference among the model results and draw useful insights into the next stage of research. • Develop detailed analysis of China's alternative transportation fuels strategies and their impact on energy consumption and GHG emissions.
Progress Report	• October: Compared the results and underlying assumptions between Ingrid Akerlind's MIT MS thesis using the FLEET model and Paul Kishimoto's MIT MS thesis using the EPPA model. • November: Compared the results and underlying assumptions between Tsinghua's 2012 China Automotive Energy Outlook report using the TCAEM model and Ingrid Akerlind's thesis using the FLEET model. • December: Modified and organized the available data from these research theses/reports in order to further compare these models.
Industry Collaboration	• N/A
US-China Collaboration Activities	• October & November: Attended the weekly workshops/conference calls between MIT and Tsinghua, held by the MIT China Center from the MIT Joint Program on the Science and Policy of Global Change. • December: Connected with Professor Ou and graduate students from the Tsinghua University, exchanging and discussing comparison results between FLEET and TCAEM models.
Issues of Concern	There are several differences between the assumptions (e.g. categories of vehicles included) and the vehicle fuel consumption values that we need to adjust for.
Notable Recent Achievements	None

Thrust	TA6: Energy Systems Analysis, Technology Roadmaps and Policy
Title	**Project 4.2: Roadmapping model development (Cooperative US)**
Personnel	PI –Prof. 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	As reported in the previous quarter, the next phase of work in this project builds on results obtained previously and as reported through the journal articles published in 2013. This new work critically reviews existing CVFS analytic methods in light of fundamental carbon balance considerations, paying close attention to the carbon stock and flow impacts of substituting biofuels for petroleum-based fuels. A new draft paper entitled, "The Liquid Carbon Challenge: Evolving Views on Transportation Fuels and Climate," was prepared and submitted to a journal for peer-review. The work re-examines the foundations of existing methods for transportation fuel lifecycle analysis (LCA; also known as fuel cycle analysis, FCA) as it has been implemented in commonly used models such as GREET. Such models form the foundation of LCA-based policies such as the Renewable Fuel Standard (RFS) and California's Low-Carbon Fuel Standard (LCFS), and FCA has long been used by DOE for program evaluation and planning. The new paper provides an in-depth review of the evolution, structure and key features of these methods; it includes over 100 citations to the literature and compares FCA to other analytic methods including terrestrial resource analysis, IPCC accounting methods, and integrated assessment modeling (IAM). A presentation of key results from this work-in-progress was made at DOE HQ on Dec. 12, 2013. The draft has also been uploaded to the CERC-CVC site for parallel review by CERC researchers and partners, and shared directly with key FCA experts at ANL, DOE, EPA, CARB and other institutions. Work in the first quarter of 2014 will involve responding to review comments received on this paper as well as making additional presentations about the work and its implications, including participation on a fuels policy panel at the upcoming SAE Government-Industry meeting in Washington, DC, on January 23.
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 Activities	No direct collaborations underway.
Issues of Concern	None.
Notable Recent Achievements	Submission of "The Liquid Carbon Challenge: Evolving Views on Transportation Fuels and Climate" for peer review.

Thrust	TA6: Energy Systems Analysis, Technology Roadmaps and Policy
Title	**Project 5: Electricity and material sourcing scenario analyses to guide vehicle technology strategies (Cooperative US)**
Personnel	PIs: Gregory Keoleian (UM), Jarod Kelly (UM) Graduate Student: Joe Colett (UM) Visiting Scholar: Lingjun Song (Beihang University) Collaborator: Hewu Wang (THU)
Objective	• Conduct materials sourcing studies to understand how vehicle life cycle energy and emissions can be impacted by the source of vehicle component material • Analyze the impact of alternative design and technology strategies for improving PHEV performance across electric grid scenarios • Develop an enhanced electrical grid model to include future fueling scenarios with renewable energy and lower carbon-based electricity strategies • Evaluate renewable electricity scenarios including renewable portfolio standards within the U.S. in the context of PHEV use and penetration • Provide guidance on vehicle technology strategies by integrating the enhanced electrical grid model and materials sourcing scenarios within a single cohesive framework

Progress Report	• October
	  o Revise aluminum journal article to focus on new electricity allocation protocols *(Achieved)*
	  o Compose second draft of PHEV-40 hood case study journal article *(Achieved)*
	• November
	  o Submit aluminum sourcing article to Journal of Industrial Ecology for review *(Achieved)*
	  o Present work to academic and industrial colleagues in CERC TA6 and monthly meeting *(Achieved)*
	  o Present work to academic and industrial advisors of the University of Michigan's Center for Sustainable Systems *(Achieved)*
	• December
	  o Defend masters thesis based on aluminum and electricity material sourcing scenario analyses *(Achieved)*
	  o Complete final preparations for PHEV-40 hood case study journal article *(Achieved)*

Industry Collaboration	• Presented results, methodology, sensitivity analysis, and new electricity allocation protocol to colleagues from the Ford Motor Company, Delphi, Saudi Aramco, U.S. Environmental Protection Agency, and Sandia National Labs
US-China Collaboration Activities	• Visiting scholar from Beihang University is being trained in LCA methods and interacting with Prof. Chris Mi at UM-Dearborn to complete an LCA study of wireless vehicle charging.
Issues of Concern	• The current GSRA (Joe) graduated this term and will be replaced with Arman Golrokhian. Additionally, Research Scientist Kelly is leaving UM for Argonne National Labs.
Notable Recent Achievements	• U.S. primary aluminum production journal article revised and submitted to the Journal of Industrial Ecology, PHEV-40 hood case study journal article ready for submission, and masters thesis on aluminum and electricity sourcing completed.