Orcas 2016:
International Conference on
Energy Conversion & Storage

The Friday Harbor Laboratories
Friday Harbor, Washington

September 7–9, 2016

Agenda

Wednesday, September 7

2:00 - 5:00 pm	Arrival, registration, and lunch
5:00 - 5:15 pm	Welcome and introductory remarks, Orcas 2016 Program Chairs
5:15 - 6:00 pm	**Dan Schwartz**, Clean Energy Institute *The Clean Energy Institute and Energy Research at the University of Washington*
6:00 - 7:30 pm	Dinner
7:30 - 9:00 pm	Poster session 1
9:00 pm	Reception

Thursday, September 8

7:45 – 8:30 am	Breakfast

Materials Synthesis & Characterization for Energy Harvesting & Storage

9:00 - 9:35 am	**Prashant Kamat**, University of Notre Dame *Lead Halide Hybrid Perovskites for Next Generation Photovoltaics*
9:35 - 10:10 am	**Lilo D. Pozzo**, University of Washington *Improving Molecular Modeling of Conjugated Polymers with Neutron Scattering*
10:10 - 10:30 am	Break
10:30 - 11:05 am	**Vincent Holmberg,** University of Washington *Nanocrystals and Nanowires for Batteries: A Chemical Engineering Perspective*
11:05 - 11:40 am	**Dana D. Dlott,** University of Illinois at Urbana-Champaign *Nonlinear Coherent Laser Spectroscopy of Electrochemical Processes*
11:40 - 11:55 am	Speaker panel discussion
11:55 am - 12:00 pm	Group picture
12:00 - 1:00 pm	Lunch
1:00 - 3:30 pm	Free time

Scaling & Stability of Third Generation Thin Film Photovoltaics

3:30 - 4:05 pm	**Devin MacKenzie**, University of Washington *Scaling of High Throughput, Low Carbon Footprint Processing of Next Generation Photovoltaic Films and Devices*
4:05 - 4:40 pm	**Mattias Andersson**, AIST, Linkoping University *Roll-to-Roll Printed Bulk Heterojunction Solar Cells*
4:50 - 5:25 pm	**Tim Kelly**, University of Saskatchewan *Perovskite Solar Cells: Lifetime Studies and Decomposition Mechanisms*
5:25 - 6:00 pm	**Kai Zhu**, National Renewable Energy Laboratory *Controlling Perovskite Structure and Grain Morphology for High-Efficiency Perovskite Solar Cells*
6:00 - 7:30 pm	Dinner
7:30 – 9:00 pm	Poster Session 2

Friday, September 9

7:45 - 8:30 am	Breakfast

Grid Systems & Storage Integrating Conventional & Alternative Energy Sources

9:00 - 9:35 am	**Ian Hiskens**, University of Michigan *Corrective Model-Predictive Control in Large Electric Power Systems*
9:35 - 10:10 am	**Le Xie**, Texas A&M University *A Metric and Market Construct of Inter-Temporal Flexibility in Power Systems*
10:10 - 10:30 am	Break
10:30 - 11:05 am	**Baosen Zhang**, University of Washington *Online Control of Storage*
11:05 - 11:40 am	**Ben Hobbs**, The Johns Hopkins University *Crediting Renewables in Electricity Capacity Markets: The Effects of Alternative Definitions upon Market Efficiency*
11:40 - 11:55 am	Speaker panel discussion
12:00 - 1:00 pm	Lunch and group departure

Speaker Abstracts

Lead Halide Hybrid Perovskites for Next Generation Photovoltaics

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Seog Joon Yoon and Jacob Hoffman, University of Notre Dame

Photoinduced charge separation in light harvesting materials is the primary step in light energy conversion devices. There have been significant efforts to employ semiconductor quantum dots (QD) and other semiconductor materials to develop low cost thin film photovoltaics [1]. With the emergence of highly efficient perovskite materials there is a need to understand the excited state behavior and charge separation events in these new materials [2-4]. The excited state characterization has allowed us to probe the evolution of perovskite structure from lead halide complex. Mixed halide lead perovskites (e.g.,CH3NH3PbI3-xBrx) undergo phase segregation to create Iodine-rich and Bromide-rich regions when subjected to visible irradiation. This intriguing aspect of halide ion movement in these mixed halide films can be tracked from the changes in the photoluminescence and absorption spectra. The photovoltaic performance of perovskite solar cells and tandem design for water splitting reaction [5] will also be discussed.

References

1. Kamat, P. V., J. Phys. Chem. Lett., 2013, 4, 908–918
2. Manser, J. S.; Christians, J. A.; Kamat, P. V., Chemical Reviews 2016, doi: 10.1021/acs.chemrev.1026b00136.
3. Manser, J. S.; Kamat, P. V., 2014, 8, 737–743.
4. Yoon, S. J. et al.. ACS Energy Letters 2016, 290-296.
5. Chen, Y.-S.; Manser, J. S.; Kamat, P. V.,. J. Am. Chem. Soc., 2015, 137, 974-981.

Improving Molecular Modeling of Conjugated Polymers with Neutron Scattering

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Conjugated polymer films, nanofibers, and networks can be ideal materials for the design of efficient photovoltaic devices, batteries, thermoelectric cells, light emitting diodes and other technologies. It is also recognized that the structure and dynamics of organic semiconductor materials correlates strongly with large changes in optical, electronic and mechanical properties so that their control and manipulation is essential to advancing the field. This presentation outlines recent results on the use of neutron and x-ray scattering techniques for the development of improved molecular simulation force fields and structural parameters specifically produced for conjugated polymers. We highlight the use of quasi-elastic neutron scattering (QENS) along with computationally efficient MD simulations to understand the nature of important nanoscale motions. X-ray and polarized neutron diffraction are also used to correlate experimental and model-generated polymer structures. QENS validation of MD force fields presents a unique opportunity to increase the accuracy of highly uncertain parameters used in simulation of conjugated polymers such as partial charges and backbone torsion. These parameters are currently estimated from quantum mechanical calculations such as density functional theory but, unlike many force fields for small molecules, are not parameterized with available experimental data. High variability is observed in these parameters for the small number of force fields that have been proposed in the literature. A vision for the accelerated development of accurate force fields for these classes of materials is also proposed.

Nanocrystals and Nanowires for Batteries: An Engineering Perspective

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Nanocrystals and nanowires are promising materials for high-capacity battery electrodes, but numerous challenges still remain before they can be implemented in industrially-applicable electrical energy storage devices. These nanostructured materials have short internal diffusion pathways, possess robust mechanical characteristics, and can be processed in either liquid dispersion or solid/powder form. Nanocrystals and nanowires are especially promising as conversion electrode materials, as they can more easily accommodate the large stresses, strains, and volume changes associated with the dramatic structural transformations that occur as the electrode repeatedly expands andcontracts with each charge-discharge cycle. Nanowires, in particular, lend themselves to new types of electrode form-factors, such as flexible ceramic fabrics that could be used in niche applications like flexible batteries. However, many significant barriers tocommercialization remain, including issues with cycling stability, rate capability, volumetric capacity, large irreversible capacity loss during the formation of the solid-electrolyte interphase (SEI) layer, electrolyte stability, current-matching, and high costs associated with the synthesis of suitable materials. Nevertheless, it is important to note that nanocrystals and nanowires are well-defined systems that can be engineered to serve as model platforms to address critical fundamental issues such as the composition and stability of the SEI layer, electrochemical potential, and constraints related to phase transformations, reaction **kinetics, and ion** and electron transport. The talk will give a broad overview of some of the materials challenges associated with electrical energy storage, and provide a perspective on the prospects, problems, and progress associated with the use of nanocrystals and nanowires in high-performance batteries.

Nonlinear Coherent Laser Spectroscopy of Electrochemical Processes

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Natalia Garcia Rey, Shuichi Toyouchi, and Alexander Moore, University of Illinois

I will briefly describe our spectro-electrochemical apparatus that uses a femtosecond laser as an in situ probe of electrochemical processes. I will summarize recent results regarding SEI formation on a Li-ion anode and low overpotential CO2 reduction. Finally I will discuss recent progress in our efforts to study fundamental mechanisms of ultrafast electrochemical processes.

Scaling of High Throughput, Low Carbon Footprint Processing of Next Generation Photovoltaic Films and Devices

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This talk will outline critical issues to be overcome in order for emerging photovoltaics (PV) technologies and their process approaches. The focus will be on a discussion of how to progress from sub-centimeter device studies based on low efficiency processes to scalable technologies that can exceed the performance and manufacturing limitations of conventional approaches in terms of performance, manufacturing cost and energy to manufacture. The capabilities being assembled at the University of Washington to address this issue will be outlined, including the CEI's Washington Scaleup and Characterization Testbed, the Scalable Printed Electronics and Energy Devices (SPEED) group, and the Washington Research Foundation (WRF) roll to roll printing facilities.

Example critical scientific and engineering research issues to be addressed in the field include increasing deposition and thermal-processing rates for PV devices, developing printable PV cathodes and the elimination of multistep lithography and depositions to form single device layers. Specific examples of work from our group in high throughput solution-based deposition, thermal conversion and crystallization of low defect perovskite films in a roll to roll process environment, new approaches to roll-to-roll processed cathodes for process-sensitive perovskite devices, and direct roll-based nanomanufacturing of efficiency-enhancing antireflective and self cleaning coatings will be presented.

Roll-to-Roll Printed Bulk Heterojunction Solar Cells

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An increased production of renewable energy is, for a variety of reasons, highly desirable. Although there are many possible applications for organic photovoltaics (OPV), compelling arguments can be made that large-scale energy production is a very viable target for the technology. The same arguments also provide very strong suggestions about where OPV needs to go in order to be successful. Early large-scale production efforts highlight several areas that require further development. Interestingly, those areas are not necessarily conventional OPV-topics, but rather related to e.g. processability and mechanical properties. An attempt will be made to demonstrate how, provided some of the key issues can be solved, OPV should be able to realize its potential and become a major contributor to the global energy production. Among the topics that will be discussed are; manufacturing capacity and its demands on the device architecture, inter-layer adhesion, intra-layer structural integrity, and electrode choices.

Perovskite Solar Cells: Lifetime Studies and Decomposition Mechanisms

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Solar cells based on lead halide perovskites have recently emerged at the forefront of solution-processable photovoltaic devices, with power conversion efficiencies over 22% having now been certified. In this presentation, I will discuss our research group's work in the area of perovskite solar cells, with an emphasis on our most recent efforts probing device failure mechanisms using fully in situ and in operando hard X-ray scattering techniques.

Controlling Perovskite Structure and Grain Morphology for High-Efficiency Perovskite Solar Cells

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Organic-inorganic hybrid halide perovskites (e.g., CH3NH3PbI3 or MAPbI3) have recently emerged as a new class of light absorbers that have demonstrated a rapid progress for solar cell applications. The certified solar conversion efficiencies have reached >22% for a small-area (~0.1 cm2) device and close to 20% for a device with 1-cm2 active area. Despite the rapid progress demonstrated by these light absorbers, there is still a lack of understanding of some fundamental material/physical/chemical properties of these materials. In this talk, I will present our recent studies toward a better understanding and control of perovskite nucleation, grain growth, and microstructure evolution using solution processing [1,2,3]. The precursor chemistry and growth conditions are found to affect significantly the structural and electro-optical properties of perovskite thin films. A nonstoichiometric precursor with excess organic salt (e.g., MAI) is found to improve perovskite film quality with enhanced crystallinity and grain size. We also found a simple post-growth MABr treatment to the perovskite MAPbI3 thin films can induce substantial grain coarsening via Ostwald ripening, leading to much improved film quality regardless of the initial film quality (e.g., pinholes and grain size). Thus, this new chemical approach enhances processing tolerance to the initial perovskite film quality and improves the reproducibility of device fabrication. The impact of grain boundary and grain size on charge transport and recombination properties will be discussed. In addition, I will briefly discuss our recent investigation on stabilizing perovskite structures by tuning tolerance factor through solid state alloying [4]. These results and others will be discussed.

References
[1] M. Yang, Y. Zhou, Y. Zeng, C.-S. Jiang, N. P. Padture, K. Zhu, Adv. Mater. (2015) 27, 6363.
[2] Y. Zhou, M. Yang, S. Pang, K. Zhu, N. P. Padture, J. Am. Chem. Soc. (2016) 138, 5535.
[3] M. Yang, T. Zhang, P. Schulz, Z. Li, G. Li, D. H. Kim, N. Guo, J. J. Berry, K. Zhu, Y. Zhao, Nat Commun (2016), 7, 12305.
[4] Z. Li, M. J. Yang, J. S. Park, S. H. Wei, J. J. Berry, K. Zhu, Chem. Mater. (2016) 28, 284.

Corrective Model-Predictive Control in Large Electric Power Systems

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Longer-term corrective control of electric power systems calls for methods that coordinate the response of diverse resources, including energy storage, demand response, fast-acting generation and FACTS devices. Model-predictive control (MPC) has shown great promise for accommodating these resources in a corrective control framework that exploits the thermal overload capability of transmission lines to limit detrimental effects of contingencies. Voltage magnitudes and reactive power are incorporated into the system model utilized by MPC in order to provide a more accurate prediction of system behavior and enable more effective control decisions. Performance of this enhanced MPC strategy is demonstrated using a model of the Californian power system containing 4259 buses. Sparsity in modelling and control actions must be exploited for implementation on large networks. A method for identifying the most effective controllable resources to enact in response to a contingency will be discussed. The proposed MPC corrective control algorithm fits naturally within energy management systems where it can provide feedback control or act as a guide for system operators by identifying beneficial control actions across a wide range of devices.

A Metric and Market Construct of Inter-Temporal Flexibility in Power Systems

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Joint work with Anupam Thatte, Yuanyuan Li, Jae-Yong An, and P. R. Kumar

The increasing penetration of variable and uncertain generation from renewable resources poses a challenge for balancing the power system supply and demand. In this paper an operational flexibility metric called lack of ramp probability (LORP) is proposed for the real-time economic dispatch. Further, a two-step robust optimization based framework is introduced to simultaneously guarantee LORP flexibility metric and ensure ramp deliverability in a multi-zonal setting. Resources such as demand response can be incorporated for providing such flexibility. We examine such a metric and market construct based on empirical data collected from Texas.

Online Control of Storage

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In this talk we consider the control of storages in power systems. This is a challenging problem because storage operations are strongly coupled over time where past actions influence future states of the system. We analyze this online problem, where decisions are made with imperfect knowledge of the future, and present some results on optimal online algorithms under storage energy constraints and nonlinear degradation cost functions. We illustrate these algorithms with an application of using storage in data centers in electricity regulation markets.

Crediting Renewables in Electricity Capacity Markets: The Effects of Alternative Definitions upon Market Efficiency

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Cynthia Bothwell, Ph.D. Student
Benjamin F. Hobbs (speaker), Founding Director, Environment, Energy, Sustainability & Health Institute
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Capacity payment mechanisms have been created in several electric power markets because of concerns that energy-only markets would not sufficiently support generation investment. As the penetration of intermittent renewable energy in electricity markets grows, there is increasing need for capacity markets to account for the contribution of renewables to system adequacy. An important issue is the definition of capacity credits for resources whose availability may be limited. Inconsistencies in capacity counting methods used by system operators motivate this investigation into the market efficiency of renewable capacity credits.

Inaccurate credits can distort investment between renewables and nonrenewables, and also among different types and locations of renewables. Using Texas (ERCOT) data, we use a model of equilibrium generation investment and operation to quantify generation mixes under different credit systems. Confirming other analyses, we find that the marginal contribution declines with renewable penetration. The loss of efficiency from inaccurate credits can be as much as 0.37% of total generation costs, which is substantial in markets whose volume runs into several tens of $billions. The inefficiency almost doubles for more ambitious renewable portfolio standards, such as those recently adopted in California and Oregon. A least-cost capacity market design should reward marginal capacity contributions by different resources considering how renewable penetration affects the timing of load peaks, net of renewable contributions.

Poster Abstracts

Photovotaics /Optoelectronics:

Decision Trees and Random Forests for Photoluminescence Prediction, Wesley Beckner
Direct Nanoimprint of Silica Sol-Gel Materials for Use in Antireflection Coating, Holly Brunner
Solar Cells From Inks: Robust Growth of Dense CZTSSe Absorber Layers, James Clark
Challenges in ZnTe/CdSe Heterojunction Nanorod Synthesis, Michael Enright
Correlating Microscale Luminescent and Photovoltaic Heterogeneity in Perovskite Solar Cells, Giles Eperon
Imaging the Potential Profile of an Ionically Conducting Polymer by Frequency Modulated-Scanning Kelvin Probe Microscopy (FM-SKPM), Lucas Flagg
Understanding the Degradation of High Performance Benzodithiophene Donor Polymers: a Pathway to More Stable Organic Solar Cells, Sarah Holliday
C-H Functionalization Towards Organic Electronic Materials, Lauren Kang
Spatially Resolved Electrical, Structural, and Chemical Properties of Hybrid Perovskite Thin Films, Jessica Kong
Self-Assembly Amphiphilic Block Copolymers for Efficient Aqueous-Processed Hybrid Solar Cells, Junhuan Li
Single-Particle Photoluminescence and Delayed Luminescence of Colloidal CuInS2 Nanocrystals, Arianna Marchioro
Fabrication of Electrodes for Solar Cells Using Photonic Curing, Deepakkrishna Mathavakrishnan
Kinetically Controlled Synthesis of Inpznse Alloyed Quantum Dots, Beth Mundy
Computational Studies of the Electronic Structures of Copper-Doped CdSe Nanocrystals, Heidi Nelson
Investigating Heterogeneous Carrier Lifetimes on the Nanoscale Using Scanning Probe Microscopy, Jake Precht
Preventing Exciton-Charge Annihilation Through Spatial and Spectral Separation, Emily Rabe
Changes in Grain Orientation Between Slot Die and Spin Coated Perovskite Layers, Brandon Rotondo
Tunable Emission of InP Quantum Dots via Post-Synthetic Modification, Jenny Stein
Solvent Effects on π-Conjugated Polymer Selectivity in Organic Nanowire Self-Assembly, Wesley Tatum
Formation of Large Grain Cation Alloyed Iodide Perovskite Films and Their Deployment in Solar Cells, Gabriella Tosado
Ferroelectric Domains Correlate with Charge Extraction in Perovskite Thin Films, Sarah Vorpahl
Force Field Development for Conjugated Polymers: Optimization with Scattering Methods, Caitlyn Wolf
Directed Assembly of Conjugated Polymers Under Electric Field, Yuyin Xi

Electroabsorption Spectroscopy Studies of the Exciton Binding Energy in the Perovskite CH3NH3PbI3 and Charge Transfer Excitons in Organic Semiconductors, Mark Ziffer

Catalysis/Surface Chemistry:

Potentiometric Titrations for Measuring the Capacitance of Colloidal Photodoped ZnO Nanocrystals, Carl Brozek
Identification of Ultrafast Electron Dynamics in Carbon Nitride, a Metal-Free Photocatalyst, Kathryn Corp
Effect of Ligand Stripping on WSe2 for the Hydrogen Evolution Reaction, Danielle Henckel
Active Membrane Architectures for Energy, Bruce Hinds
Metal Selenide Nanostructures for Hydrogen Evolution, Olivia Lenz
Surface Redox Reactivity of Colloidal Nanocrystals, Emily Tsui
Effect of Surface Ligands on Co/CoP for the Hydrogen Evolution Reaction, David Ung
Kinetic Rate Studies of CO2 and H2O Co-Electrolysis on Solid Oxide Electrodes, Jonathan Witt
Peptide Enabled Addressable Immobilization of Kinetically Matched Fusion Enzymes in Membrane Flow Bioreactors, Deniz Yucesoy

Battery:

LiOx Deposits on a Pt Tip, Understanding the Fundamentals of Li-O2 Batteries, Kelly Carpenter
Accelerating Battery Research with Benchtop Advanced X-ray Spectroscopies, Evan Jahrman
Printable Flexible Zinc Air Battery, Taichong Ma
Unlocking Insight into Battery Systems with Nonlinear Electrochemical Impedance Spectroscopy (NLEIS), Matthew Murbach
Printed, Nontoxic Metal-Air Batteries for Flexible Electronics, Caleb Ogier
Self-Learning Battery Management Systems for Li-ion Batteries, Manan Pathak
Application of Battery Modeling in Electrode Design, Yanbo Qi
The Influence of Electric Field on Lithium-Oxygen Battery Cathode Reactions, Honorio Valdes

Grid:

Applications of a Multi-Agent Based Platform for Optimal Battery Management and PV Based Voltage Control in a Campus Distribution Grid, Rémy Rigo-Mariani
A Bi-Level Optimization with Model Predictive Control for Operation of Building Thermal Loads in a Transactive Framework, Rémy Rigo-Mariani
Decentralized Coordination of a Building Manager and an Electric Vehicle Aggregator, Jesus Contreras Ocana
Campus Energy Testbed: Battery Energy Storage System (BESS) Based Photovoltaic Charging Station (PV-CS) for a Green University Transportation, Agata Swierc
Look-Ahead Bidding Strategy for Energy Storage, Yishen Wang
Economic Dispatch of Battery Energy Storage in Electric Energy Markets, Bolun Xu

Photovotaics /Optoelectronics

Decision Trees and Random Forests for Photoluminescence Prediction

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High performance computing and machine learning engender new strategies to engineer materials. By creating automated, adaptive experimental architectures, previously insermountable design spaces can be considered. This work illustrates the performance of random forests as implemented in the scikit-learn package in python at predicting photoluminescence for perovskite solar cells. The poster presents a tutorial that is a creative exploration space for introducing other researchers to one of the most commonly used machine learning algorithms.

Direct Nanoimprint of Silica Sol-Gel Materials for Use in Antireflection Coatings

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Optical antireflection coatings (ARCs) are of significant research interest due to their wide array of applications in photovoltaic devices, electronics, optical equipment, and display glass. While many varieties of ARCs have been researched, one of the largest tasks left to accomplish is to develop an optimized coating that is cost-effective, durable, and manufacturable. It has been shown that a close-packed array of nanostructures results in a uniform and effective ARC by creating a gradient of material at the surface. This gradient leads to a gradual transition in the effective index of refraction which results in minimized reflection. Previous research has shown the successful single step imprinting of non-durable polymers or an unscalable multi-step process using silica based materials. This research attempts to develop a thixotropic silica sol-gel to allow for single step nanoimprinting of a durable ceramic material for use in a roll-to-roll printing process. We have successfully synthesized silica sol-gels in a variety of viscosities and thixotropic behaviors. These gels have been blade coated and directly imprinted with a nanopillar array through a manual imprinting process. The printed coatings have been imaged in an SEM and the results show successful nanopattern transfer in many samples. Future work includes experimenting with the addition of silica nanoparticles to try and further enhance the thixotropic quality of the gel. The importance of developing this process goes beyond the present ARC applications as advances in printed nanostructured dielectric materials could significantly impact research in printed 2D photonic devices and tandem solar cells.

Solar Cells From Inks: Robust Growth of Dense CZTSSe Absorber Layers

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Kesterite Cu2ZnSn(S,Se)4 (CZTSSe) based thin-film solar cells are one of the most exciting prospects for inexpensive photovoltaic electricity generation due to their tunable, optimal band gap of 1-1.5 eV and earth-abundant, low-toxicity materials. Of the deposition techniques available for CZTSSe, solution processing is attractive because of high material utilization and scalability. While a wide variety of CZTSSe solution routes have been explored, one of the most successful routes at producing high efficiency devices utilizes DMSO as a solvent with metal chloride and acetate salts complexed with thiourea. Using this green, low-toxicity molecular ink process we have produced devices with power conversion efficiencies (PCEs) reaching 11.8%, which are approaching the record CZTSSe device efficiency of 12.6%. Other groups have used this DMSO ink process to make CZTSSe devices, but many have seen bi-layer or tri-layer absorber morphologies associated with lower fill-factor and PCE. In this study we utilize glow-discharge optical emission spectroscopy (GDOES) to demonstrate that multi-layer morphologies are strongly tied to the thermal annealing profile of the ink before selenization. During annealing acetate, thiourea, and chloride decompose into gaseous products. When these films are selenized unconverted carbon, nitrogen, and chloride containing compounds become trapped in the film, which inhibits grain growth and leads to unwanted multi-layer morphologies. By generating films with a range of thermal profiles and comparing their GDOES profiles, morphologies, and device IV performance we have determined transport rates of unwanted species out of the film, allowing us to avoid multi-layer morphologies, and generate high PCE devices.

Challenges in ZnTe/CdSe Heterojunction Nanorod Synthesis

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Colloidal nanoscale semiconductors are promising materials for solar energy conversion due to their low cost solution processability, absorption profile in the visible region of the electromagnetic spectrum, and tunability of optical and electronic properties as a function of size and surface chemistry. In particular, type II anisotropic double-heterojunction rod structures facilitate charge separation after photoexcitation, leading to prolonged exciton lifetimes. An attractive nanomaterial is CdSe/ZnTe/CdSe, a heterojunction nanorod that confines excited electrons to CdSe nanorod ends and holes to the ZnTe core. Despite the potential for CdSe/ZnTe/CdSe nanorods to improve charge separation, the one-pot approach to synthesizing these materials is obstructed by cation exchange. Cadmium molecular species (i.e. cadmium phosphonate and cadmium oleate) in the presence of ZnTe will readily exchange with the zinc in the nanomaterial to generate (Zn,Cd)Te alloys, even when selenium precursors are included in the synthetic procedure to encourage CdSe growth. This cation exchange process is facilitated by rapid cadmium coordination to the surface of the ZnTe nanorod followed by subsequent incorporation of cadmium into the nanorod while zinc ions are extracted. The rate and extent of cation exchange is directly correlated to the temperature of the experiment. The reaction's temperature and cadmium ion concentration dependence are examined to better evaluate the kinetic and thermodynamic properties of cation exchange processes as well as understand conditions to be aware of when designing heterojunction growth syntheses.

Correlating Microscale Luminescent and Photovoltaic Heterogeneity in Perovskite Solar Cells

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Whilst perovskite solar cells have demonstrated an unprecedentedly rapid rise in power conversion efficiencies to over 21%, they are still far off their theoretical maximums of >30%.1 Recently, several reports have emerged demonstrating that there is significant heterogeneity in the microscale properties of perovskite films – some grains seem to be of higher material quality than others, and grain boundaries show high densities of non-radiative defects.2,3 It has been suggested that this heterogeneity could limit the performance of solar cells made from these films. However, a direct link between film heterogeneity and device performance has not been shown.

Here, we probe heterogeneity on the microscale in full solar cell devices using a series of in-situ electrical and photophysical measurements, and show a direct link to solar cell performance for the first time. Using high-resolution spatially resolved luminescence mapping and laser beam induced current and voltage mapping, we find that there is significant variation in the photovoltaic performance of state-of-the-art perovskite solar cells across the device on the scale of microns. We correlate regions of high and low voltage and current (and hence PCE) with their luminescent efficiencies, and elucidate the impact that these regions have on photovoltaic performance.

We go on to show that certain passivation techniques can affect this device performance heterogeneity, with the most promising techniques showing fewer 'dark' grains and correspondingly higher photovoltaic performance. Based on our results we elucidate rational routes to pushing the performance of perovskite solar cells close to the thermodynamic limits.

Imaging the Potential Profile of an Ionically Conducting Polymer by Frequency Modulated-Scanning Kelvin Probe Microscopy (FM-SKPM)

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Ionically conducting polymers are currently being investigated for a wide variety of energy applications, especially as solid state electrolytes for batteries and fuel cells. Here we investigate the system of bis(trifluoromethane) sulfonamide lithium salt (LiTFSI) dissolved into poly(ethylene oxide) (PEO). Using AC impedance spectroscopy, we measure the conductivity of this system as a function of lithium salt concentration. We then use frequency modulated – scanning kelvin probe microscopy (FM-SKPM) to examine the voltage potential across a ~10 μm wide junction between two gold electrodes deposited on top of the PEO:LiTFSI samples. A negative bias is applied to one of the gold electrodes while the other electrode is grounded. We find that when there is no lithium salt in the system the voltage is dropped evenly over the width of the junction. However, in systems with lithium salt the voltage profile shows a steep drop close to the negatively charged electrode. Furthermore, as the concentration of lithium salt increases the location of this potential drop moves further from the electrode edge.

Understanding the Degradation of High Performance Benzodithiophene Donor Polymers: a Pathway to More Stable Organic Solar Cells

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Christine Luscombe, University of Washington

Organic solar cells have the potential to substantially reduce the cost of solar energy production relative to their traditional inorganic counterparts, thanks to their lower materials costs and compatibility with solution-processed, large-area printing techniques. In recent years, significant research efforts have focused on increasing the power conversion efficiency of these devices, especially in the development of sophisticated new donor polymers that can capture more of the solar spectrum and promote a more favorable charge transporting network in the device. Polymers based on the benzo[1,2-b:4,5-b']dithiophene repeat unit have been among the most successful, with efficiencies of over 11% published using these materials. However, much less attention has been paid to the fact that many of these devices require strictly inert conditions for processing, and can degrade rapidly during operation due to issues of photo-oxidative stability with the polymers. It is therefore crucial to develop more stable donor polymers in order to realize a low-cost, printable technology with practical operating lifetimes. There is currently very little consensus on the actual mechanism by which such polymers degrade, due to a lack of standardized measurements in the literature, however there is some evidence to suggest that the solubilizing side-chains play a crucial role in initiating the photo-oxidative degradation process. We therefore present a side-by-side study featuring two high performance benzodithiophene-based polymers named PTB7 and PTB7-Th, which differ only in their pendant side-chains. By systematically investigating the degradation of polymers under illumination in air, using a range of chemical, optical and photovoltaic characterization methods, we attempt to define the mechanism of degradation in these polymers, which can in turn help in the development of more air- and light-stable derivatives to advance this technology.

C-H Functionalization Towards Organic Electronic Materials

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Jason A. Lee, Christine K. Luscombe, University of Washington

Our group works on improving current conjugated polymer synthesis techniques, specifically in the form of arylation methods, to find ways that C-H functionalization can supplement or improve existing methodologies. Presented here are two projects describing our efforts in seeking out and adopting new pathways for conjugated polymer synthesis with efforts towards more facile steps, lower costs, and more environmentally-friendly processes.

Spatially Resolved Electrical, Structural, and Chemical Properties of Hybrid Perovskite Thin Films

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Thin film organic-inorganic perovskite semiconductors are highly heterogeneous materials on the nanoscale. One of the major roadblocks to the material's commercialization is its stability. Here, we use photoluminescence (PL) microscopy and time-resolved electrostatic force (tr-EFM) microscopy to look at changes in the PL and charging rates of a film as it photodegrades. Following a film's electrical and structural properties as it does so can provide insight on its degradation mechanism. While we can study its electrical and structural evolution, due to the limits of optical spectroscopy, deriving corresponding chemical information has been significantly more difficult. However, the recent development of a photoinduced force microscope (PiFM) presents the ability to spatially correlate chemical, electrical, and structural properties of these materials. The PiFM probes a photoinduced force gradient, allowing for direct, non-destructive molecular identification. Applications of PiFM in the context of hybrid perovskite thin films will also be presented.

Self-Assembly Amphiphilic Block Copolymers for Efficient Aqueous-Processed Hybrid Solar Cells

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Due to their low cost and environmental friendliness, aqueous-processed polymer/nanocrystal hybrid solar cells (HSCs) have attracted much attention in recent years. In this work, water-soluble hybrid materials consisting of amphiphilic block copolymers (ABCPs) and CdTe nanocrystals (NCs) were used as active layers to fabricate the HSCs via aqueous process. The ABCPs containing poly(3-hexylthiophene) (P3HT) could self-assemble into ordered nanostructured micelles, which further transform to nanowires by co-micellization with homo-P3HT additives. The hybrid materials formed an interspersed network after high temperature annealing. A power conversion efficiency up to 4.82% was achieved. The properties of the hybrid materials and the film morphology were further studied and correlated to the device performance. The aqueous-processed HSCs based on the ABCPs and NCs offer a clean and effective method for the fabrication of highly efficient solar cells.

Single-Particle Photoluminescence and Delayed Luminescence of Colloidal CuInS2 Nanocrystals

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CuInS2 nanocrystals (NCs) have recently attracted interest as nontoxic alternatives to CdSe, PbS, and related semiconductor NCs for numerous nanophosphor applications. The large photoluminescence (PL) Stokes shifts and long lifetimes of CuInS2 NCs make them particularly attractive emitters for applications in bioimaging, light-emitting diodes, and luminescent solar concentrators. Determining the details of the luminescence mechanism in CuInS2 NCs is of fundamental importance for optimizing their performance in technological applications.

Single-nanocrystal spectra and blinking measurements on CuInS2 semiconductor nanocrystals will be presented. We will show that luminescence bandshapes are broad compared to those typical of individual II–VI or related semiconductor nanocrystals. This finding is similar to what has been observed in ensemble measurements, and consistent with the hypothesis of strong electron–phonon coupling in the emissive excited state of these CuInS2 semiconductor nanocrystals.

Ensemble luminescence measurements reveal the existence of a long-lived excited state in these nanocrystals that continues to emit photons over several orders of magnitude in time following the excitation pulse. This delayed luminescence overlaps in time and shows similar distributed kinetics to the blinking “off” times of the same nanocrystal sample, suggesting that these two phenomena arise from the same microscopic carrier-trapping and detrapping processes. Further evidence of this proposal is given by excitation power dependence measurements, where the delayed luminescence saturates at very low emission intensities under the excitation power densities used in the single-nanocrystal measurements. This finding is consistent with the metastable charge-trapped state associated to delayed luminescence being the “off” state of the luminescence blinking cycle.

Fabrication of Electrodes for Solar Cells Using Photonic Curing

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Photonic curing is the process of curing a specimen by utilizing the light energy absorbed by it. Samples like uncured silver nanoparticles absorb most of the light in the solar spectrum and get cured. Flashing light of similar spectrum with very high intensity would instantly cure them. Moreover the substrates, that do not absorb most of the emitted wavelengths, will not be affected, since each pulse locally heats only the silver nanoparticles for a few milliseconds. The main objective of the work is to cure the silver nanoparticles faster and also in a way that does not damage the substrates below it. The process utilizes xenon flash lamps to cure silver nanoparticles coated/Inkjet printed on Glass or PET. The resistivity of the sample cured by photonic flashes for 2 seconds is 24000 times lower than uncured samples and 2.5 times greater than thermally sintered samples for 30 mins. This is a drastic reduction in curing time for appreciable reduction in resistivity. Photonic curing is preceded by solvent evaporation which takes 15 minutes. To make the whole process completely scalable a conveyor toaster was utilized to evaporate the solvent which reduced the time to 30 seconds. This will reduce the production time of solar cells and hence it helps in the scalability and the cost reduction of the process. Photonic sintering would be a wonderful replacement for the traditional thermal sintering in scalable processes like roll to roll printing.

Kinetically Controlled Synthesis of Inpznse Alloyed Quantum Dots

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Quantum dots have had some commercial success as high quantum yield color-pure emitters for display technologies. However, broader application is limited by the use of cadmium based materials which exhibit significant toxicity and necessitate the development of different, less toxic materials. InP and its alloys have been touted as viable alternatives to CdSe quantum dots due to their optical properties. InPZnSe quantum dots have been synthesized utilizing selenourea-based precursors of varying reactivities that allow for a range of monomer release rates to be accessed. By altering the reactivity of the precursor, the size of the nanocrystals and composition of the alloy can be tuned. The as-synthesized alloyed particles exhibit a range of photoluminescence properties from exclusively trap emission to fully band edge recombination. The alloys will ultimately be shelled with ZnS to access Cd-free emitters with high photoluminescence quantum yield over a range of visible wavelengths.

Computational Studies of the Electronic Structures of Copper-Doped CdSe Nanocrystals

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Copper-doped nanocrystals (NCs) are a class of materials with great potential as phosphors in applications ranging from luminescent solar concentrators to energy-efficient lighting. To understand the intrinsic advantages and limitations of these materials, the electronic structures of copper-doped CdSe NCs are investigated using time-dependent density functional theory. Comparison of the electronic structures of Cu+- and Cu2+-doped NCs indicates that only the Cu+ ground state is consistent with the experimental absorption and photoluminescence (PL) spectra of copper-doped NCs, Cu2+-doped NCs being characterized by low-energy charge-transfer and d-d excited states that quench visible PL. In the luminescent metal-to-conduction-band charge-transfer (MLCT) excited state of the Cu+-doped CdSe NCs, the photogenerated hole is calculated to be localized at the copper dopant. Strong electron-phonon coupling in this MLCT excited state causes substantial geometric distortion along totally symmetric and Jahn-Teller nuclear coordinates, with a correspondingly large excited-state nuclear reorganization energy. This excited-state nuclear reorganization causes the broad PL bandshape and large PL Stokes shift observed experimentally. Singlet and triplet MLCT excited-state configurations are also examined computationally. The sign and strength of the computed magnetic exchange coupling between the conduction-band electron's spin and the copper-localized spin are both consistent with experimental results. These calculations yield fundamental insights into the electronic structures and photophysical properties of copper-doped semiconductor NCs relevant to their potential application as spectral conversion phosphors in lighting and solar technologies.

Investigating Heterogeneous Carrier Lifetimes on the Nanoscale Using Scanning Probe Microscopy

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We study surface photovoltage decays on nanosecond time scales using intensity-modulated scanning Kelvin probe microscopy (IM-SKPM). Previous experiments within our group have shown that IM-SKPM probes charge carrier recombination rates with a spatial resolution of < 50 nm and a temporal resolution of 500 μs. IM-SKPM's carrier lifetime maps are not diffraction limited and thus provide more detailed information than traditional photoluminescence mapping.

Here we show how we can improve IM-SKPM's temporal capabilities by several orders of magnitude, allowing us to study systems with lifetimes as short as 10 ns. We envisage these improvements to allow us to construct carrier lifetime maps for emerging thin film photovoltaic systems such as hybrid organic-inorganic perovskites and copper zinc tin sulfide.

Preventing Exciton-Charge Annihilation Through Spatial and Spectral Separation

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Plastic electronics such as organic solar cells, organic semiconductor lasers, and organic light emitting diodes all operate under conditions in which there may be a significant spatial and energetic overlap between bound excitons and free charge carriers. The exciton-charge coexistence can result in annihilation reactions forming highly excited charge carriers, leading to significant chemical degradation in many cases. Here, we propose a method to reduce losses due to exciton-charge annihilation in a model subphthalocyanine (SubPc) organic solar cell material by spectrally shielding the diffusion of excitons from the transport of charge carriers. We are exploring 1:1 blends of SubPc and hole-conducting materials, where the ionization potential energies (IP) and excited state electron affinities (EA*) are precisely tuned such that excitons would remain unquenched on SubPc while free charge carriers re-locate onto the hole conductor. In addition to this spatial exciton-charge separation, we hypothesize that exciton-charge annihilation could be mitigated by energetic separation between the SubPc exciton emission and the hole conductor charge absorption. We demonstrate with solution-phase spectroelectrochemistry that tris(4-carbazoyl-9-ylphenyl)amine (TCTA) meets these requirements for shielding SubPc excitons. Additionally, we propose straightforward methodology for confirming the effect of hole transfer and exciton shielding with thin-film devices using a combination of charge-modulation spectroscopy and voltage-dependent photoluminescence. We believe these results have future implications for materials design strategies aimed at controlling exciton-charge annihilation in organic electronics.

Changes in Grain Orientation Between Slot Die and Spin Coated Perovskite Layers

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To achieve an end goal production of flexible, large area, organometallic perovskite based solar cells, changes in fabrication techniques from a small research scale will have to be made. Larger scale deposition techniques of blade and slot die coating have been proposed as a simple scale up; however, changes to the materials properties as a result of differences in deposition have not been examined. To this extent, we examined changes in methylammonium lead iodide and formamidinium lead iodide perovskite grain formation utilizing 2D X-Ray Diffraction mapping to observe preferential grain orientation in both spin coated and slot die coated perovskite layers. In order to determine how changes in orientation would potentially effect photovoltaic device performance both the optical and electrical properties were characterized and compared as well.

Tunable Emission of InP Quantum Dots via Post-Synthetic Modification

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Providing energy for an expanding global population is a challenging prospect for renewable energy sources; thus, improving energy efficiency of current technologies is an important objective. One appealing option to minimize our energy consumption is to focus our efforts on improving quantum dot (QD) materials as down-conversion fluorophores for use as drop-in color filters in energy efficient solid-state lighting. QDs have proven their viability in the marketplace as attractive options for next generation displays with an improved color gamut. While CdSe has been most widely used for such down-conversion applications, indium phosphide (InP) QDs are an attractive lower-toxicity alternative to utilizing well-defined CdSe QDs as down-conversion fluorophores. However, traditional InP colloidal syntheses have photoluminescence quantum yields (PL QY) <1% and require further modification to be viable for lighting and display applications. Our investigations have demonstrated the ability of M2+ Lewis acids (M= Cd, Zn) to dramatically enhance the PL QY of InP QDs. Addition of cadmium and zinc has also been found to red- and blue-shift, respectively, the lowest energy absorption and emission of InP QDs while maintaining particle size. This treatment results in a facile strategy to post-synthetically tune the luminescence color in these materials. Optical and structural characterization (XRD, TEM, XAS, ICP) have led us to identify the primary mechanism of PL turn-on as surface passivation of phosphorus dangling bonds, affording PL QYs up to 49%. Additionally, this route to PL enhancement and color tuning may prove useful given the difficulty in synthetically accessing fluorescent InP of different sizes.

Solvent Effects on π-Conjugated Polymer Selectivity in Organic Nanowire Self-Assembly

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In semi-conducting polymers, charge carriers and excitons freely move through the system of conjugated π-orbitals. Defects in the polymer chains, such as lower regioregularity, disrupt this motion. It is classically predicted that in bulk films crystalline domains form that exclude these defects, pushing them into amorphous domains to retain perfect crystallinity. One of the main difficulties in studying the crystallization and its treatment of defects is separating the crystalline and the amorphous domains. By supersaturating solutions of poly(3-hexylthiophene) (P3HT), the participating π-orbitals attract and align with other π-orbitals either in other polymer chains or within its own chain, causing self-assembly and precipitation of micron-long wires with widths on the order of exciton diffusion lengths. Investigating these nanowires elucidates how defects within the polymer chains are incorporated into crystalline regions of bulk P3HT films because there are no amorphous regions of P3HT in the isolated nanowires. Conventional understanding of crystallization predicts that any defects within the nanowires alter both the physical dimensions and the electronic properties. Contrary to these predictions, our results show that defects are incorporated into the nanowire structures but not alter the physical dimensions of the nanowires. Further, by altering the ratio of good/poor solvent that the P3HT nanowires assemble in, polymer chains with fewer defects and a higher degree of polymerization (DP) can be preferentially incorporated into the nanowires first. As the solution ages, polymer chains with more defects and lower DP, or both, are then incorporated into these nanoscopic, crystalline domains.

Formation of Large Grain Cation Alloyed Iodide Perovskite Films and Their Deployment in Solar Cells

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Organic-inorganic halide perovskites are an exciting, emerging active layer material which has had an unprecedented increase in solar cell conversion efficiencies over the past five years. Binary lead and tin perovskite not only reduces the toxic lead content, but more importantly offers the benefits of narrower band gaps for broader adsorption of the solar spectrum and better charge transport for higher photocurrent densities. Previously, Pb-Sn perovskite fabrication used a one-step solution spin coat process which created small grains with many pinholes, affecting device performance. Our lab reports large, smooth Pb-Sn grains via a two-step solution process with thermal plus solvent vapor-assisted thermal annealing. The absorption onset was extended to 950 and 1010 nm for the CH3NH3SnxPb1-xI3 perovskites with x = 0.1 and 0.25, respectively. The highest PCE of 10.25% was achieved from the planar perovskite solar cell with the CH3NH3Sn0.1Pb0.9I3 layer prepared via the DMSO vapor-assisted thermal annealing. The next step was creating a PbI2-(DMSO) complex to implement a DMSO exchange with MAI for a more efficient fabrication. To create the Pb-Sn perovskites, 10% of tin was added to the PbI2-(DMSO) solution. These results support that the higher affinity of Sn-O allowed the tin to swap positions with lead, creating an effective template for the DMSO intermolecular exchange. In the future, we hope to optimize our solar cell architecture with this new Pb-Sn perovskite intermolecular exchange process creating a new way to control and manipulate film morphology, gran size and distribution of metal cations in binary perovskite layers.

Ferroelectric Domains Correlate with Charge Extraction in Perovskite Thin Films

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Perovskites have emerged as the most promising new material for light harvesting applications with rapid gains in efficiency being achieved in only the last several years. However, several open questions about fundamental material properties of perovskites remain, including the presence of ferroelectric domains and what role they play in device performance. This work shows that a) ferroelectric domains do exist in both hybrid inorganic-organic and inorganic perovskite films and that b) charge extraction is correlated with domain orientation under operating conditions. We employ piezoresponse force microscopy (PFM) and photoconductive atomic force microscopy (pcAFM) to investigate different formulations of hybrid and inorganic perovskite thin films using a multimodal AFM approach. We use lateral and vertical PFM (LPFM and VPFM) to characterize both in-plane and out-of-plane piezoelectric domain orientations. We correlate these images with pcAFM, a contact AFM technique that maps local conductivity under light bias using a conductive probe. We find that, on the nanoscale, domain orientation is directly connected to charge extraction in both hybrid methylammonium lead triiodide and inorganic cesium lead triiodide films, with in-plane domains dominating in higher efficiency films.

Force Field Development for Conjugated Polymers: Optimization with Scattering Methods

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Organic photovoltaic (OPV) performance relies on optoelectronic properties of conjugated polymers. These devices have greater flexibility than more prevalent inorganic solar cells and use lower-cost roll-to-roll fabrication. However, efficiencies remain low, limiting their adoption. Increased control over the molecular structure and dynamics of conjugated polymers can be used to improve charge transport properties of the material and reach higher device efficiencies. Computational methods can also be employed to guide the design of new organo-electronic materials, but accurate and reliable force fields still need to be produced. In this work, we focus on identifying key parameters essential for the development of force fields that accurately capture the effects of electronic conjugation. Structure and dynamics are explored by means of wide-angle x-ray scattering (WAXS) and quasi-elastic neutron scattering (QENS), respectively. These results, combined with density functional theory, are used to optimize molecular dynamics simulations and fine-tune simulation force fields. A challenge is this method is computationally expensive and data intensive, resulting in an inefficient force field development process. Machine learning will be employed in the future to automate and accelerate this step. Here, we present work on the model conjugated polymer, poly(3-hexylthiophene) (P3HT), where we assess the quality of uncertain force field parameters such as partial charges and torsion potentials. Furthermore, we extend this work to more complex polymers that lack suitable simulation force fields: P3DDT, PQT-12 and PBTTT. In the future, the accelerated development of accurate force fields for conjugated polymers will enable in-silico discovery of better performing materials.

Directed Assembly of Conjugated Polymers Under Electric Field

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Anisotropic structure is desirable in organic electronics to facilitate charge transport. It can also induce the polarization of light to realize opto-electronic devices. Electric field alignment is a promising method because it is economical, easily tunable and scalable. In this work, it is shown that the poly(3-hexylthiophene) (P3HT) can be aligned in both micro- and nano-meter scale. The effect of amplitude, frequency, level of supersaturation and polymer concentrations are systematically investigated. The optimum condition for alignment is determined utilizing optical microscopy, small angle neutron scattering (SANS) and atomic force microscopy (AFM). The polymer chain orientation is characterized by x-ray diffraction (XRD) experiment and the stacking direction is along the electric field lines. The dominating mechanism is proposed to be dielectrophoresis and self-assembly. The mechanical and electrical properties, probed by rheology and impedance spectroscopy measurement, are enhanced after alignment. The feasibility of aligning other thiophene based polymers is also explored. The effect of polymer side chains and backbones on the electric field alignment is revealed, which is crucial for the design of new polymers that will result in well controlled uni-directional structures for applications in OPVs, OLEDs and OFETs devices. The results demonstrate an alternative method to direct the growth of conjugated polymers, which has a strong potential to be economically integrated into the large scale process of organic electronics.

Electroabsorption Spectroscopy Studies of the Exciton Binding Energy in the Perovskite CH3NH3PbI3 and Charge Transfer Excitons in Organic Semiconductors

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We use electroabsorption (EA) spectroscopy to study the electronic properties associated with primary optical transitions in hybrid organic-inorganic perovskites and semiconducting polymers. In the perovskite CH3NH3PbI3, we study the second harmonic EA spectra at the fundamental absorption edge and establish that the room temperature EA response follows the low-field Franz-Keldysh-Aspnes (FKA) effect. Following FKA analysis we measure values for the exciton binding energy (7.4 meV), the electron-hole reduced effective mass (0.12 ± 0.03 m0), and the one-electron band gap (1.633 eV) [1]. In organic donor-acceptor (DA) bulk heterojunction blends, we study the sub-optical gap EA signal in order to reconstruct the charge-transfer state absorption spectrum by means of a classic Stark effect analysis [2]. We apply this technique to reconstruct the CT absorption spectrum in non-fullerene DA blend systems, in which CT absorption is otherwise undetectable using standard methods [3]. Finally, in neat polymer systems we use EA to measure values for the change in dipole moment and change in polarizability between ground and excited state with regards to primary excitonic transitions. In contrast with previous studies, we find that the magnitude of ground-to-excited state dipole moment change does not necessarily dictate charge separation efficiency.

[1] Ziffer, M. E., et al. ACS Photonics 3, 1060-1068, doi:10.1021/acsphotonics.6b00139 (2016)
[2] Bublitz, G. U. & Boxer, S. G. Annu. Rev. Phys. Chem. 48, 213-242, doi:10.1146/annurev.physchem.48.1.213 (1997).
[3] Vandewal, K. Annu. Rev. Phys. Chem. 67, 113-133, doi:10.1146/annurev-physchem-040215-112144 (2016)

Catalysis/Surface Chemistry

Potentiometric Titrations for Measuring the Capacitance of Colloidal Photodoped ZnO Nanocrystals

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Colloidal semiconductor nanocrystals offer a unique opportunity to bridge molecular and bulk semiconductor redox phenomena. Here, potentiometric titration is demonstrated as a method for quantifying the Fermi levels and charging potentials of free-standing colloidal n-type ZnO nanocrystals possessing between 0 and 20 conduction-band electrons per nanocrystal, corresponding to carrier densities between 0 and 1.2×1020 cm−3. Potentiometric titration of colloidal semiconductor nanocrystals has not been described previously, and little precedent exists for analogous potentiometric titration of any soluble reductants involving so many electrons. Linear changes in Fermi level vs charge-carrier density are observed for each ensemble of nanocrystals, with slopes that depend on the nanocrystal size. Analysis indicates that the ensemble nanocrystal capacitance is governed by classical surface electrical double-layers, showing no evidence of quantum contributions. Systematic shifts in the Fermi level are also observed with specific changes in the identity of the charge-compensating counter-cation. As a simple and contactless alternative to more common thin-film-based voltammetric techniques, potentiometric titration offers a powerful new approach for quantifying the redox properties of colloidal semiconductor nanocrystals.

Identification of Ultrafast Electron Dynamics in Carbon Nitride, a Metal-Free Photocatalyst

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We correlate the excited state electron dynamics of graphitic carbon nitride, a metal-free photocatalyst, with hydrogen evolution efficiency. To the best of our knowledge, our work represents the first fluence-dependent, near-infrared induced absorption feature in the transient absorption spectrum of graphitic carbon nitride. The lifetime and intensity of this signal is not affected by the addition of a hole scavenger (triethanolamine). However, with the addition of an electron scavenger (sodium sulfate) we observe a significant reduction in signal intensity and a decrease in the lifetime. We conclude that this signal arises due to a photoinduced negative charge on carbon nitride. The lifetime of this signal increases after graphitic carbon nitride has been oxidized with sulfuric and nitric acid, which could be an indication that the photoinduced electron is localized on defect states in the carbon nitride matrix. Additionally acid-etched carbon nitride shows a 20% increase in hydrogen production compared to graphitic carbon nitride, relating to the increased lifetime of the photoinduced negative charge. We believe that our observation of the ultrafast excited state dynamics in carbon nitride, and how it relates to hydrogen evolution, will help provide a roadmap for structural modifications aimed at controlling charge separation lifetime and increasing catalytic efficiency.

Effect of Ligand Stripping on WSe2 for the Hydrogen Evolution Reaction

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Transition metal dichalcogenides (TMDs) are a class of material that has emerging applications in catalyzing the hydrogen evolution reaction (HER) at low overpotentials with high current densities. These materials are advantageous in that they are produced with cheaper, more earth abundant materials than precious metals like platinum, which is still the best catalyst for the HER. Catalytic performance of these materials often increases dramatically when synthesized with features on the nanoscale. One TMD that has seen some success in catalyzing the HER is WSe2. Current methods to synthesize nanoscale, catalytically active WSe2, however, require expensive synthetic techniques that are not scalable. These methods involve either lithium intercalation of bulk powder using alkyl lithium reagents or high vacuum and temperature techniques such as chemical vapor deposition. Recently we developed a colloidal synthesis of catalytically active WSe2 nanoflowers without the need for these energy intensive techniques. The colloidally synthesized nanoflowers are catalytically active for the HER and are competitive with WSe2 prepared by other techniques when a ligand stripping step is applied. The effect of this ligand stripping method are compared with other forms of ligand removal, such as annealing, to help rationalize the increased catalytic performance. The mechanism and activity of the WSe2 nanoflowers have been evaluated with a variety of electrochemical techniques in order to probe the HER activity.

Active Membrane Architectures for Energy

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Carbon nanotubes (CNT) have three key attributes that make them of great interest for novel membrane applications 1) atomically flat graphite surface allows for ideal fluid slip boundary conditions for 10,000 fold faster fluid flow 2) the cutting process to open CNTs inherently places functional chemistry at CNT core entrance for gatekeeper activity and 3) CNT are electrically conductive allowing for electrochemical reactions and application of electric fields gradients at CNT tips. Pressure driven flux of a variety of solvents (H2O, hexane, decane ethanol, methanol) are 4-5 orders of magnitude higher than conventional Newtonian flow [Nature 2005, 438, 44] due to atomically flat graphite planes inducing nearly ideal slip conditions. However this is eliminated with selective chemical functionalization [ACS Nano 2011 5 3867-3877] needed to give chemical selectivity. These unique properties allow us to explore the hypothesis of producing 'Gatekeeper' membranes that mimic natural protein channels. With anionic tip functionality strong electroosmotic flow is induced by unimpeded cation flow with similar 10,000 fold enhancements [Nature Nano 2012 7 133-39]. With enhanced power efficiency, carbon nanotube membranes were employed as the active element of a switchable transdermal drug delivery device that can facilitate more effective treatments of drug abuse and addiction [PNAS . 2010 107 11698]. Applications in energy storage and water treatment and active membrane systems [Adv. Funct. Mater. 2014 24 4317] are also discussed.

Metal Selenide Nanostructures for Hydrogen Evolution

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We have developed a method for synthesizing (W/Mo)Se_2 nanostructures via a colloidal method that demonstrate high catalytic activity for the hydrogen evolution reaction. We discuss the impact of solvent, ligand choice, and post-processing steps on the structure and activity of the (W/Mo)Se_2 catalyst. Notably, we demonstrate a large reduction in overpotential at 10 mA/cm^2 with a simple chemical stripping of surface capping ligands that can be done at room temperature.

Surface Redox Reactivity of Colloidal Nanocrystals

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Overcoming carrier trapping at the surfaces of nanocrystals is one of the major challenges in the development of nanocrystal devices for display, solar cell, and energy applications. Understanding the structural and compositional origin of mid-gap surface states is expected to lead to improved methods for removing or mitigating the traps. Here, we use a combination of photochemical electronic doping, spectroscopy, and electrochemical methods to control and observe carrier trapping and delocalization in colloidal semiconductor nanocrystals. We show that photodoping of CdSe nanocrystals proceeds via a dark pre-reduction step followed by electron transfer to the valence band hole. These photodoped conduction-band electrons decay slowly under anaerobic conditions to surface electron trap states, with trapping governed by nanocrystal surface composition.

Effect of Surface Ligands on Co/CoP for the Hydrogen Evolution Reaction

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Surface ligands are a ubiquitous trait of all colloidally synthesized nanoparticles. The surface ligands stabilize the surface of the nanoparticles and prevent agglomeration. The identity of these ligands has a huge range, including but not limited to amines, phosphines, and carboxylates. Generally, these ligands are thought to inhibit the activity of the particles for hydrogen evolution because they occupy active sites. However, there is no known direct correlation between type of surface ligand and its affect on catalysis. In this study, we are interested in studying how the identity of the surface ligand affects cobalt and cobalt phosphide nanoparticles' activity for the hydrogen evolution reaction.

Kinetic Rate Studies of CO2 and H2O Co-Electrolysis on Solid Oxide Electrodes

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Recent advances in carbon capture create new opportunities for recycling CO2 into liquid fuels to store intermittent electrical energy. One option is to co-electrolyze CO2 and H2O at high temperature using solid oxide electrolysis cells (SOECs). Although promising, the factors controlling rates of CO2 and H2O reduction in SOECs are not well understood, hampering development. Traditional electrochemical techniques have difficulty resolving the various kinetic and transport rates. This can be overcome through the use of differential electrochemical mass spectroscopy coupled in-operando with linear and non-linear electrochemical impedance spectroscopy (EIS and NLEIS) to study co-electrolysis on representative materials such as CeO2 and LaSrCrMnO3. EIS can measure overall rates but NLEIS can identify the details of the reaction mechanisms through its non-linear responses. As a result of coupling gas phase and electrochemical responses, the rate laws of the various reaction occurring on and around the surface will be differentiated.

Peptide Enabled Addressable Immobilization of Kinetically Matched Fusion Enzymes in Membrane Flow Bioreactors

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Biomimetic reconstruction of metabolic pathways by incorporating multiple enzymes and relevant cofactors in confined environments holds tremendous promise for sustainable green synthesis of fine chemicals and developing efficient biomolecular devices. The major challenge in designing such systems is to control spatial organization of multiple biological components in sequentially with high spatial precision. GEPI tags (genetically engineered peptides for inorganic solids) have emerged as novel surface functionalization moieties because of their exquisite molecular recognition properties. These solid-binding peptides are ideal candidate as a molecular linkers to immobilize biomolecules on variety of solid surfaces. Here, we use GEPIs as molecular linkers to demonstrate addressable co-immobilization of two enzymes, formate dehydrogenase and lactate dehydrogenase, spatially immobilized on gold and Ni-NTA activated AAO-membrane in a flow reactor. The work highlights the utility of GEPI as genetic linker and molecular erector for addressable immobilization of multiple enzymes. The principles laid out in this study can be applied to other enzymes and extended into reconstructing more sophisticated enzymatic biosensors and biofuel cell devices.

Battery

LiOx Deposits on a Pt Tip, Understanding the Fundamentals of Li-O2 Batteries

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Lithium-oxygen batteries are theoretically many times more energy dense than current lithium-ion batteries. Research on the Li-O2 batteries has been promising, yet leaves a myriad of unanswered questions. Limited information is currently known about the elementary mechanistic steps in Li-O2 battery chemistry. As a result, lack of cell reversibility and electrolyte degradation are two commonly reported and vaguely understood problematic phenomena. A fundamental investigation to identify and study the relevant reactions is required to establish a working understanding of the kinetic and energetic basis of the complex battery chemistry. Only then can battery design improvements be made. Research conducted outside of a working battery is needed to decouple and understand individual mechanisms.

Surface science experiments are proposed and run under ultra-high vacuum (UHV) using field ionization microscopy (FIM) to probe the oxygen reduction and evolution reactions (ORR, OER) that occur on the cathode of Li-O2 batteries. FIM investigates reactions on an atomically sharp platinum field emitter tip. The Pt hemispherical tip is ideal for modeling the many micro-facets found on a Pt electrocatalyst. Additionally, the high fields required for FIM mimic those typically found within a working battery. The FIM system molecularly monitors surface reactions to provide data on the evolution and morphology of LiOx species. The attached mass spectrometer characterizes intermediates and products and allows for calculation of individual species coverage. Change of coverage with field and temperature, which are precisely controlled, lead to reaction thermodynamic calculations.

Accelerating Battery Research with Benchtop Advanced X-ray Spectroscopies

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Until recently, advanced x-ray spectroscopy remained largely the sole domain of synchrotron facilities. While national-lab scale sources provide the ultimate in technical capability, the present access model is necessarily restrictive to the point of slowing progress on critical projects and nearly prohibiting more routine analytical characterization. Over the last three years, our group at the UW has been developing new families of lab-based instruments for x-ray absorption fine structure (XAFS) and high-resolution x-ray emission spectroscopy (XES).

This poster addresses the hard x-ray XAFS user facility for battery research at the UW, the Seidler group's ongoing research with hard x-ray XES as a new high-throughput tool for metal speciation, and the development of a novel XES system capable of fitting inside a glove box for air-sensitive studies. Selected applications will include redox flow batteries, Li-ion batteries, and progress toward studies of Li-S batteries with the miniature XES system.

Printable Flexible Zinc Air Battery

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In this work, we present a paradigm to print flexible zinc air batteries layer by layer. Screen printed silver ink was used as the current collector for both anode and cathode. The electrolyte is Ionic Liquid/PVA gel which is blade coated on the anode. The hydrophilic ionic liquid does not evaporate during further annealing and helps absorb water from the atmosphere. The air cathode is made of screen-printed carbon nanotubes which are decorated by Cobalt Oxide graphene composite. The total thickness of the battery is roughly 0.5mm. The thin film battery has a capacity of 1mh/cm2. The working voltage is 0.87 voltage at 0.05mA/cm2 currently. The batteries also show no performance changes under bending condition. Making batteries can be fabricated by a layer-by-layer printing strategy dramatically increase the production rate of flexible batteries.

Unlocking Insight into Battery Systems with Nonlinear Electrochemical Impedance Spectroscopy (NLEIS)

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Electrochemical impedance spectroscopy (EIS) is widely used in the study of lithium ion batteries due to the relative ease of using equivalent circuit analogs to extract kinetic/transport parameters and provide data for health prognostics. Application of a small perturbation restricts EIS to probing only the linear regime despite the inherently nonlinear nature of the electrochemical system. While this linearization leads to a relatively straightforward analysis (a large reason for the widespread adoption of the technique), the degeneracy of linearized EIS signals can result in a loss of discriminating power and artificially limit the informational content of the technique.

Here we present an extension of traditional small amplitude EIS measurements – called nonlinear EIS (NLEIS) – in which the nonlinearity of a lithium ion battery is probed by measuring the higher harmonic response to moderate amplitude perturbations. To avoid the degeneracy of equivalent circuit analogs, a physics-based impedance model is used to analyze the nonlinearly generated harmonics. Exploring the parameter space of the models enables an analysis of the sensitivity of different physicochemical parameters (and interactions between parameters) across a range of perturbation frequencies. We discuss the insight gained through these techniques into the most sensitive experimental measurements for extracting information related to particular processes or states of interest and discuss the increased informational content in nonlinear impedance measurements.

Printed, Nontoxic Metal-Air Batteries for Flexible Electronics

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Next generation wearable electronics such as glucose-sensing contact lenses and electrotactile stimulation devices require energy storage that is thin, flexible, high-capacity, reliable and safe. Al-air and Zn-air batteries are promising due to their high specific energies (400 Wh/kg and 1090 Wh/kg, respectively), stability, and low toxicity compared to Li-ion batteries (265 Wh/kg). High-precision, 3D extrusion printing is used to assemble batteries on flexible circuits by consecutive deposition of anode, electrolyte, and oxygen electrocatalyst inks. Polymer binders and conductive nanoparticle fillers allow these layers to bend without fracturing or loss of conductivity and enhance their print characteristics. Due to the nature of flexible electronics, algorithms are needed for adjusting print routines to account for geometric deviations in the substrates onto which the batteries are fabricated based on laser scan data. The ability to print batteries directly onto devices negates the need for interconnections, allowing new age electronics to be more reliable, scalable, compact and inexpensive while affording engineers unprecedented freedom in their designs.

Self-Learning Battery Management Systems for Li-ion Batteries

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Battery Management Systems (BMS) are critical to the performance of lithium-ion batteries in any application, ranging from cell phones to EVs to giant batteries in an electric grid. An efficient BMS should be able to accurately predict the internal states of the battery such as the Sate-of-Charge (SOC), State-of-Health (SOH) using the Voltage and current measurements from the battery, along with maintaining safe operations of the battery. The accurate determination of these internal states holds the key for the optimal performance of batteries. The effect of inaccurate state estimation leads to conservative use of batteries and at worst, may cause potentially unsafe situations leading to thermal runaway. This necessitates the development of accurate models that could predict different states of the battery more accurately, which at the same time are not as computationally complicated to be deployable in current BMS.

Here we present an approach to optimally manage the batteries based on adaptive physics-based models, that is chemistry agnostic, which can predict various parameters required for the battery model and predict optimal charging profiles in real-time.

Application of Battery Modeling in Electrode Design

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With the widespread of electronic devices and the employment of energy storage systems for renewable energy and electric vehicles, the needs for batteries that can meet different requirements are surging. However, the performance of lithium-ion batteries today still needs to be improved to fully meet the requirements of these applications. Model-based battery design is an efficient method to address this issue. Methods and approaches developed to improve the performance of a given chemistry are valid and applicable for next-generation chemistry if the approach has a solid fundamental basis. No matter what material we end up using, it is always necessary to optimize the cell design to fully utilize that material. In this poster, a migration model with nonlinear reaction kinetics was developed, instead of the linear kinetics reported in the literature. The optimal uniform porosity of 0.42 was predicted by this model. In addition, optimization with respect to porosity distribution as a function of distance from the current collector was explored, so as to further improve the electrochemical performance. Furthermore, a porous electrode model for the positive electrode with concentration gradient was developed, and used to maximize specific energy under different discharge rates. The results suggest that we need different battery designs for different applications.

The Influence of Electric Field on Lithium-Oxygen Battery Cathode Reactions

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In recent years, lithium-air batteries have attracted significant interest due to increased energy density compared to currently available technologies such as lithium-ion batteries. However, issues such as loss of capacity and high charging overpotentials due to irreversible reactions in the cathode have limited their commercial deployment. Recent work has focused in solving these issues and understanding the processes occurring in the cathode. Most studies involve electrochemical cells with subsequent cathode characterization. However, the complexity of electrochemical cells complicates gaining further insight. An alternative involves ultrahigh vacuum (UHV) surface science studies. The effects of electric field (and potential) on kinetics can be studied in a UHV system based on field ionization microscopy (FIM) using Pt field emitter tips as substrate. The surface electric field is easily controllable by biasing the tip at voltages around 5 kV. Reactions are carried out by adsorption of the species of interest followed by application of a baseline field. Adsorbed reaction products (LiOx) and their morphology can be monitored by FIM, while reaction intermediates can be detected by field desorption (FD). In this work, the formation of LiOx deposits as a function of field, temperature, and coverage are studied with FIM and FD. Reactions are conducted on both Pt and carbon-coated Pt tips, the latter to simulate a cathode. The differing field dependencies of LiOx deposit formation for different x will be used to estimate relative rates of LiOx formation.

Grid

Applications of a Multi-Agent Based Platform for Optimal Battery Management and PV Based Voltage Control in a Campus Distribution Grid

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Developed by the Pacific Northwest National Laboratory (PNNL) VOLTTRON is a multi-agent execution platform dedicated to power systems. This open source and modular software supports the communication between different entities over the grid. This presentation will describe two examples of agent development and software interactions for power management in a campus distribution grid. A first experiment optimizes the operation of an energy storage system based on a lithium-ion battery. An optimization is performed using a rolling window with a periodic refreshment of the forecasts for both production and consumption. The objective is to minimize the electrical bill while reducing the peak power and responding to incentives. The second application controls grid voltages using smart micro inverters for PV panels. The power factor of the inverters is periodically adjusted using either a greedy method or a modified power flow while maximizing the active power produced.

A Bi-Level Optimization with Model Predictive Control for Operation of Building Thermal Loads in a Transactive Framework

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It has been extensively proven that smart controls of building loads and especially the Heating, Ventilation and Air-Conditioning (HVAC) can enhance power systems management and facilitate energy saving as well as the integration of renewables. In addition to conventional demand response programs, a new paradigm called “transactive control” has emerged. This paradigm relies on market mechanisms in a multi-agent framework. This presentation will describe the implementation of this framework using a bi-level optimization and considering the HVAC of an existing building. On the end-user side a multi steps ahead optimal control performs arbitrage between cost, comfort and the ability to respond to transactive signals. On the utility side an outer optimization loop is introduced to find the most appropriate price signal to send to the building in order to follow a predefined power profile. In addition an artificial neural network is used to implement the Model Predictive Control (MPC) while a finer model in EnergyPlus simulates the controlled building and allows computing the prediction error. Simulations are performed with different settings of the building. Finally, a case with several buildings is investigated.

Decentralized Coordination of a Building Manager and an Electric Vehicle Aggregator

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Flexibility in the power system is essential if we want to accomplish ambitious renewable energy goals. The ability to control commercial buildings and electric vehicles (EVs) is a promising source of demand flexibility. In some cases, buildings and EVs share common infrastructure (e.g a transformer) or interact with each other to accomplish a goal (e.g. reduce local peak demand). In such cases, the building and EV demand scheduling problems are effectively a single demand scheduling problem. Ideally, it would be solved as a single optimization problem. However, doing so might not be possible due to a number of concerns (e.g data privacy). This paper proposes the use of the Dantzig-Wolfe decomposition to solve the building-EV demand scheduling problem in a decen- tralized fashion. The effectiveness of the proposed methodology is demonstrated in three case studies where the building and EV problems are coupled by either: i) demand limits, ii) a peak demand charge, or an iii) itemized billing tariff. Results show that the optimal solution can be reached while sharing a minimal amount of information.

Campus Energy Testbed: Battery Energy Storage System (BESS) Based Photovoltaic Charging Station (PV-CS) for a Green University Transportation

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With the trends encouraged by governments and political parties to increase the adoption of Renewable Energy Sources (RES); solar energy, and in particular photovoltaics (PV), is poised as an excellent candidate to offset the energy requirements of charging stations (PV-CS) for Electric Vehicles (BEV). This work presents a 10.5 kW Transient System Simulation (TRNSYS) model of a university campus PV-CS to determine sizing as well to determine the best operating strategies for a Battery Energy Storage System (BESS). The economical optimization model is formulated via theoretical approach adopting the Simple Payback Period (SPP) indicator. The optimization takes into account the campus transportation load profile while BESS is used to attain the shortest SPP. The results, from both theoretical as well as simulation approach, reveal that leveraging the campus BEVs charging via BESS based PV-CS scheme has the potential to reduce the energy demand from the grid, and to maximize self-consumption efficiency.

Look-Ahead Bidding Strategy for Energy Storage

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As the cost of battery energy storage continues to decline, we are likely to see the emergence of merchant energy storage operators. These entities will seek to maximize their operating profits through strategic bidding in day-ahead electricity market. One important parameter in any storage bidding strategy is the state-of-charge (SoC) at the end of the trading day. Because this final SoC is the initial SoC for the next trading day, it has a strong impact on the profitability of storage for this next day. This paper proposes a look-ahead technique to optimize a merchant energy storage operator's bidding strategy considering both the day-ahead and the following day. Taking into account the discounted profit opportunities that could be achieved during the following day allows us to optimize the SoC at the end of the first day.

We formulate this problem as a bi-level optimization. The lower level problem clears a ramp-constrained multi-period market and passes the results to the upper level problem which optimizes the storage bids and offers. Linearization techniques and KKT conditions are used to transform this non-linear and non-convex mathematical problem with equilibrium constraints (MPEC) into an equivalent single level MILP problem. Numerical results obtained using the RTS system demonstrate the benefits of the proposed look-ahead bidding strategy and the importance of considering ramping and network constraints.

Economic Dispatch of Battery Energy Storage in Electric Energy Markets

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The integration of grid-scale battery energy storage (BES) increases power system renewable penetrations. However, current dispatch methods of BES are not economical because the strong causality between battery lifetime and cycle depth of discharge are not reasonably priced in existing market models. This poster demonstrates a new BES market dispatch model based on electrochemical battery degradation mechanisms. We demonstrate the proposed model in a full-year BES dispatch simulation using ISO New England market price data. Model performance and accuracy are evaluated with respect to different number of linearization blocks. Simulation results show that the proposed BES model can significantly prolong the lifetime of battery cells and improve the profitability of BES in electric energy markets.


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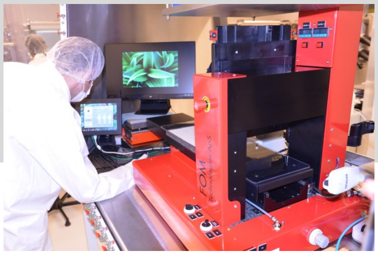

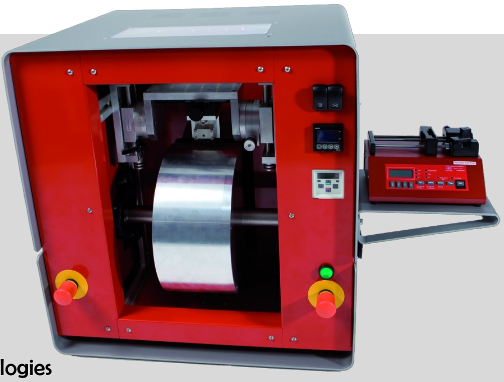

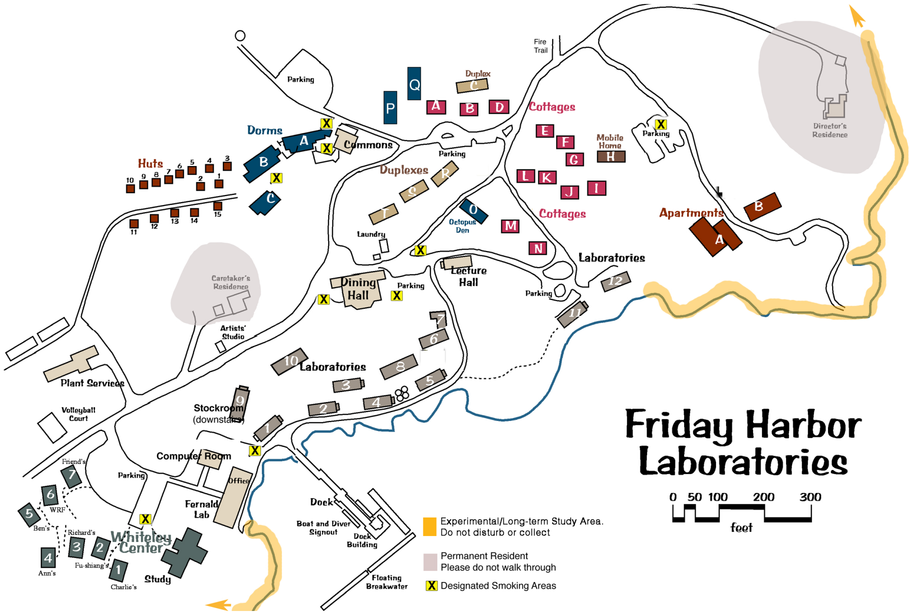

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