Argonne NATIONAL LABORATORY

Annual Postdoctoral Research and Career Symposium

October 8, 2015

Argonne National Laboratory Postdoctoral Research and Career Symposium

October 8, 2015

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2015 Postdoctoral Research and Career Symposium
October 8, 2015

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2015 Postdoctoral Research and Career Symposium
October 8, 2015
TCS Conference Center
Agenda

8:00 am — Continental Breakfast, Registration and Poster Setup

Morning Session

8:30 am — Welcome Remarks from Lisa Durham, Director, Argonne Leadership Institute, Argonne National Laboratory

8:45 am — Keynote Address by Careers Program Manager, American Physical Society

9:15 am — Panel Discussion "CV through Your Future Employer's Eyes"

Representatives from:

Academia: Tim Marin, Associate Professor, Benedictine University
Saw-Wai Hla, Professor, Ohio University (Joint Appointment with Argonne National Laboratory Center for Nanoscale Materials)

Industry: Rick Weber, Founder and President, Materials Development, Inc.
Tim Emmerling, Recruiter, Allstate Insurance Company

Lab: Seth Snyder, Water Initiative Leader, Argonne National Laboratory

10:45 am — Collaboration Talk by Volker Rose, Physicist, Argonne National Laboratory

11:15 am — Lunch Pickup and Company Booth Setup

Networking Lunch

11:30 am — Networking Lunch Kickoff by Chris Kramer, Manager, Media Relations and External Affairs, Argonne National Laboratory

11:45 am — Networking Lunch—Participants will meet with representatives from companies and various organizations/institutions during this session

11:45 AM – 12:15 PM	Table 1
12:15 PM – 12:45 PM	Table 2
12:45 PM – 1:15 PM	Table 3

Afternoon Session

1:15 pm — Flash Talks

1:30–4:30 pm — Networking Reception and Company Booth Time (Room 1416)

1:30 pm — Poster Session A (Rooms 1404–1407)

2:30 pm — Poster Session B (Rooms 1404–1407)

3:30 pm — Poster Judging Scoring

4:30 pm — Closing Remarks by Al Sattelberger, Deputy Director for Programs, Argonne National Laboratory

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2015 Postdoctoral Research and Career Symposium
October 8, 2015

2015 Keynote Address

Breaking the Myth of "Non-Traditional" Careers: The Real Story About Employment for Science Graduates

Dr. Crystal Bailey, Careers Program Manager, American Physical Society (APS), College Park, MD

Dr. Crystal Bailey is the Careers Program Manager at the American Physical Society (APS) in College Park, MD. Bailey works on several projects geared toward marketing physics and physics career information to high school students, undergraduates, graduate students, and physics professionals. Some of her principal projects include the Physics InSight slide show, Future of Physics Days events for undergraduates at the APS annual meetings, the APS Job Board and Job Fair, APS webinars, and maintaining resources on the APS Careers website. She also devotes significant amounts of time to planning career workshops and other professional-development-related activities to support early-career physicists and helps manage the activities of the APS Committee on Careers and Professional Development.

Before coming to the APS, Bailey did research in nuclear physics at Indiana University (IU), Bloomington, in the area of few-body systems. In 2008 she received the Konopinski Award for Outstanding Graduate Teaching from the IU Physics Department. She graduated with a PhD from IU in 2009.

Welcome Remarks

Lisa Durham, Director, Argonne Leadership Institute, Argonne National Laboratory

Lisa Durham provides strategic direction and management of the Argonne Leadership Institute. She develops, implements, and administers innovative and creative programs designed to cultivate the leadership potential of all employees and enable them to maximize their unique contributions to science, engineering, and Argonne's mission. Lisa received her B.S. in geology from Texas A&M University and her M.S. in geosciences from Purdue University. She began her career as an environmental engineer and has spent 28 years at Argonne, responsible for programs, projects, and research associated with geo-environmental analyses. She is a member of Argonne's Women in Science and Technology (WIST) steering committee, which works to recruit, retain, and promote women; she is a member of the Diversity and Inclusion Advisory Council and a chairperson for numerous outreach activities. She is a recipient of the 2012 WIST Diversity Award and is a University of Chicago Strategic Laboratory Leadership Program participant.

Career Skills Panel:

CV through Your Future Employer's Eyes

Tim Marin, Associate Professor,
Benedictine University

Saw-Wai Hla, Professor, Ohio University
(Joint Appointment with Argonne National Laboratory
Center for Nanoscale Materials)

Rick Weber, Founder and President,
Materials Development, Inc.

Tim Emmerling, Recruiter,
Allstate Insurance Company

Seth Snyder, Water Initiative Leader,
Argonne National Laboratory

Collaborative Talk:

Don't Worry, Be Social: Why Science Is More Fun through Collaborations

Volker Rose, Physicist

Volker Rose received a doctoral degree from RWTH Aachen University in Germany in 2005. He started his career as a postdoc at Argonne National Laboratory. He became a staff scientist in 2007, with an interdivisional appointment at both the Advanced Photon Source and the Center for Nanoscale Materials. As a physicist, his research has touched the realm that encompasses our cultural heritage; for example, he has investigated the chemical makeup of the paints used by Picasso and of 160-year-old daguerreotypes (the world's first practical photographic technique) and planet-friendly, concrete building materials in the form of geopolymers. In 2012, Volker Rose was awarded the prestigious DOE's Early Career Research award, with $2.5 million in funding to develop the synchrotron x-ray scanning tunneling microscope, a novel high-resolution microscope that can be used for imaging nanoscale materials with chemical, electronic. and magnetic contrast. In his upcoming talk, he will highlight the importance of collaboration in building a fruitful career.

Networking Lunch Kickoff

Christopher J. Kramer, Manager, Media Relations and External Affairs, Argonne National Laboratory

Christopher J. Kramer is the Manager of Media Relations and External Affairs for Argonne. He has more than 30 years of experience in the field.

He is adept at leading and managing national and regional relations and at directing internal and external communication programs to promote knowledge, awareness, and support for multifaceted issues and programs. He is an internationally known risk and crisis communication expert who has assisted hundreds of local, state, federal and international agencies in preparing for how to effectively communicate during a time of crisis.

He served for 10 years as Public Information Officer for the State of Utah Department of Public Safety. He also served as Lead Public Information Officer for security at the 2002 Olympic Winter Games.

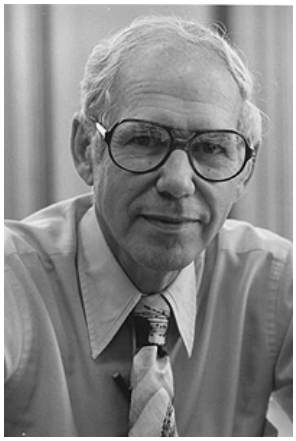
Closing Remarks

Dr. Al Sattelberger, Deputy Director for Programs, Argonne National Laboratory

Alfred P. Sattelberger is the Deputy Laboratory Director for Programs at Argonne National Laboratory. He is responsible for the management and integration of the laboratory's science and technology portfolio, strategic planning, and the Laboratory Directed Research and Development (LDRD) program. Sattelberger has been at Argonne since 2006 and has served as the Associate Laboratory Director (ALD) for Physical, Biological and Computing Sciences, ALD for Physical Sciences, ALD for Energy Engineering and Systems Analysis, and Interim ALD for Applied Sciences and Technology.

Sattelberger obtained a PhD in inorganic chemistry from Indiana University and was a National Science Foundation Postdoctoral Fellow at Case Western Reserve University. Prior to joining Argonne, he was a faculty member in the Chemistry Department at the University of Michigan and a staff member at Los Alamos National Laboratory. At Los Alamos, he held several scientific management positions and was named a Senior Laboratory Fellow in 2005. His personal research interests span actinide coordination and organometallic chemistry, fundamental technetium chemistry, and metal-metal bonding and catalysis. He is a Fellow of the American Association for the Advancement of Science (AAAS) and of the American Chemical Society (ACS), the chair of the Chemistry Section of the AAAS, a past chair of the Inorganic Chemistry Division of ACS, a member of DOE's Nuclear Energy Advisory Committee (NEAC), and chair of the Fuel Cycle Subcommittee of NEAC. He holds faculty appointments at Northwestern University and the Harry Reid Center for Environmental Studies at the University of Nevada, Las Vegas. He also lectures occasionally at The University of Chicago.

Robert G. Sachs
Award for Excellence for
Outstanding Poster Presentation



Robert G. Sachs

Robert G. Sachs (May 4, 1916 – April 14, 1999) was an American theoretical physicist. Sachs helped create Argonne National Laboratory and served as its director from 1973 to 1979. He was notable for his work in theoretical nuclear physics, terminal ballistics, and nuclear power reactors. As Associate Director of Argonne from 1964 to 1968, Sachs also determined experimental priorities for the lab's powerful new particle accelerator, the Zero Gradient Synchrotron. The Postdoctoral Society of Argonne chose to name the Award for Excellence for Outstanding Poster Presentation after Robert G. Sachs due to his early career achievements. Early in his career, Sachs established himself as an influential scholar, scientific policy maker, and research administrator.

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Poster Abstracts

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A-1

Cu_4 Nanocatalyst Assisted Conversion of Carbon Dioxide to Methanol at Low Pressures

Halder, Avik[1], Cong Liu[1], Bing Yang[1], Eric Tyo[1], Karthika L. Kolipaka[1], Soenke Seifert[2], Janae DeBartolo[2], Bernd von Issendorff[4], Peter Zapol[1], Larry A. Curtiss[1], and Stefan Vajda[1,3,5,6]

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[4] Physikalisches Institut, Universität Freiburg, 79104 Freiburg, Germany
[5] Department of Chemical and Environmental Engineering, School of Engineering & Applied Science, Yale University, New Haven, CT 06520, USA
[6] Institute for Molecular Engineering, The University of Chicago, Chicago, IL 60637, USA

CO_2 conversion to methanol under atmospheric pressures mediated by Al_2O_3-supported copper nanoclusters has been investigated. We performed a temperature-programmed reaction (TPRx) combined with in situ grazing incidence x-ray absorption near-edge structure (GIXANES) measurements. A significant rise in Cu_4 activity is observed around 225°C along with a complete reduction of primarily oxidized Cu_4 clusters. Density functional theory calculations reveal the low activation energy barrier of Cu_4 clusters for hydrogenation of CO_2 to methanol, making this the most efficient catalyst at low-pressure [1]. Extended study is pursued under concentrated CO_2 and H_2 gases where grazing-incidence small-angle x-ray scattering (GISAXS) results show signature of nano-sized assembly formation is stable at temperatures higher than 200°C but disintegrates on cooling below 150°C. This is a curious effect not observed for Cu_4 deposited on other supports like ZnO, ZrO_2 or UNCD under identical experimental conditions. We are presently exploring the support effect in Cu4 activity under concentrated reactant environment. This comprehensive experimental study supported by theoretical calculations indicates that small Cu clusters bear the potential of being an excellent catalyst for recycling released CO_2 with an activity higher than bulk Cu surfaces and large Cu nanoparticles.

Reference

1. Cong Liu, Bing Yang, Eric Tyo, Soenke Seifert, Janae DeBartolo, Bernd von Issendorff, Peter Zapol, Stefan Vajda, and Larry A. Curtiss, *Journal of the American Chemical Society* **27**, 8676 (2015).

A-2

Nonlinear Light-Matter Interaction in Semiconductor Photonic Crystals

Husko, C.[1,2], A. Blanco-Redondo[2], S. Combrie[3], M. Wulf[4], K. Kuipers[4], T.F. Krauss[5], A. De Rossi[3], and B.J. Eggleton[2]

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[3] Thales Research and Technology, 1 Av. A. Fresnel, 91767 Palaiseau, France
[4] Center for Nanophotonics, FOM Institute AMOLF, Science Park 104, 1098 XG, Amsterdam, The Netherlands
[5] Department of Physics, The University of York, York YO10 5DD, UK

Semiconductor optical waveguides have been the subject of intense study for over two decades due to the promise of unprecedented control of light in a monolithic photonic chip. In this, we focus on the nonlinear temporal dynamics in these systems which have now reached nanoscale dimensions. Critically, the ability to independently tune the dispersion and the nonlinearity in our photonic crystal waveguide samples enables our examination of completely different nonlinear regimes simply by changing the input wavelength. Our ultra-sensitive frequency-resolved electronic gating (FREG) technique and numerical algorithm are capable of extracting full temporal pulse envelope and phase information of the

sub-picojoule pulse energies. Specifically we report on experiments and theory of: (i) optical pulses in an intra-pulse plasma in silicon and GaInP photonic crystals [1, 2, 3] and (ii) temporal broadening due to nonlinear free-carrier modulation in silicon [4].

References
1. A. Blanco-Redondo, C. Husko, et al., *Nature Communications* **5**, 3160 (2014).
2. P. Colman, C. Husko, S. Combrié, et al., *Nature Photonics*, **4**, 862 (2010).
3. C. Husko, et al., *Scientific Reports* **3**, 1100 (2013)
4. A. Blanco-Redondo (C. Husko), *Optica* **5**, 299 (2014).

A-3

Magnetic Nanotube Composite Membranes

Ignacio-de Leon, Patricia, Emily Rabe, Meltem Urgun-Demirtas, Richard Brotzman*, and Xing Chen

Energy Systems Division, Argonne National Laboratory, Argonne, IL 60439
*Currently working for Materials Engineering, Motorola Mobility

Novel nanocomposite membranes, composed of magnetic nanotubes embedded in a polymer to form a permselective layer on microporous supports (e.g., polysulfone, regenerated cellulose), are reported for applications in wastewater treatment and catalytic transformation of feedstocks into products with concurrent separations. The nanotubes have diameters ranging from ca. 5–200 nm, with an aspect ratio as high as 10,000, which enables the nanotubes to function as pores, or nanochannels, that span the permselective layer thickness. The metal/metal oxide nanotubes offer key advantages: (1) hydrophilic surface provides improved antifouling properties; (2) facile nanotube alignment via an applied magnetic field during membrane formation; (3) a high density of close-packed channels for increased permeability; (4) the nanotube diameter (both inner and outer) may be tailored to enable a range of applications according to desired target compound in the feed; and (5) potential metal/metal oxide catalytic activity. Membranes are fabricated using a scalable (up to >1200 cm^2 per batch) technology on a wide-web format. Herein we demonstrate the application of our nanocomposite membranes towards the filtration of lignin, a contaminant in wastewater from paper and mill industries.

A-4

Molecular Design of Nanocrystals for Third-Generation Photovoltaics Using First Principles Simulations

Vörös, Márton[1,2], Nicholas Brawand[1], and Giulia Galli[1,2]

[1] Institute for Molecular Engineering, University of Chicago, Chicago, IL 60637
[2] Materials Science Division, Argonne National Laboratory, Chicago, IL 60439

Semiconductor nanocrystal (NC) solar cells hold the promise of delivering photoconversion efficiencies going above the Shockley-Queisser limit of ~33%. The highest delivered device efficiency to date is still at 10%, and one of main reasons for such a performance deficit is the imperfect passivation of the surface of NCs, which leads to the formation of states in their energy gap. Such states may act as recombination centers. We developed a density-functional-theory-based method to compute nonradiative recombination at defects at the surface of NCs [1]. We found that dangling bonds at the surface of oxidized silicon NCs can indeed efficiently capture charges and that engineering the strain at the interface of the NCs and their embedding matrix would reduce the nonradiative recombination rate. Instead of trying to eliminate gap states, one may turn their presence into an advantage. According to the intermediate band (IB) paradigm,

a suitably positioned IB within the band gap of the absorber would allow for absorbing photons with below band-gap energy, thereby increasing the photocurrent. In our recent work, we proposed that colloidal NCs films composed of doped surface reconstructed CdSe NCs would provide an ideal platform for implementing the IB paradigm [2].

References
1. Nicholas P. Brawand, Márton Vörös, and Giulia Galli, *Nanoscale* **7**, 3737 (2015).
2. Márton Vörös, Giulia Galli, and Gergely T. Zimanyi, *ACS Nano* **9**, 6882 (2015).

A-5

An Electrodynamics-Langevin Dynamics (ED-LD) Approach to Simulate Metal Nanoparticle Interactions and Motion

Sule, N.[1], S.A. Rice[1,2], S.K. Gray[3], and N.F. Scherer[1,2]

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[3] Center for Nanoscale Materials, Argonne National Laboratory, Argonne, IL 60439

Understanding the formation of electrodynamically interacting assemblies of metal nanoparticles requires accurate computational methods for determining the forces and propagating trajectories. However, since computation of electromagnetic forces occurs on femtosecond timescales, simulating the motion of colloidal nanoparticles on milliseconds to seconds timescales is a challenging multi-scale computational problem. Here, we present a computational technique for performing accurate simulations of laser-illuminated metal nanoparticles. In the simulation, we self-consistently combine the finite-difference time-domain method for electrodynamics (ED) with Langevin dynamics (LD) for the particle motions. We demonstrate the ED-LD method by calculating the 3D trajectories of a single 100-nm-diameter Ag nanoparticle and optical trapping and optical binding of two and three 150-nm-diameter Ag nanoparticles in simulated optical tweezers. We show that surface charge on the colloidal metal nanoparticles plays an important role in their optical self-assembly. In fact, these simulations provide a more complete understanding of the assembly of different structures of two and three Ag nanoparticles that have been observed experimentally, demonstrating that the ED-LD method will be a very useful tool for understanding the self-organization of optical matter.

A-6

Engineering Nanofluid Electrodes: Control of Rheology and Electrochemical Activity of Nickel Hydroxide Nanoparticles

Sen, Sujat[1], Elahe Moazzen[2], Chun Man Chow[1], Carlo Segre[2], and Elena Timofeeva[1]

[1] Energy Systems Division, Argonne National Laboratory, Argonne, IL 60439
[2] Department of Physics & CSRRI, Illinois Institute of Technology, Chicago, IL 60616

Nanofluid electrodes or nanoelectrofuels have significant potential in the field of flow batteries, as at high loadings of solid battery active nanoparticles, their energy density can be orders of magnitude higher than in traditional redox flow battery electrolytes. Requirements to nanofluid electrodes are that they must have a manageable viscosity at high particle concentrations (i.e., easily pumpable) and exhibit good electrochemical activity towards charge and discharge reactions. Engineering of such nanofluid electrodes involves development of new and unique approaches to stabilization of nanoparticle suspensions. In this work, we demonstrate a surface modification approach that allows controlling the viscosity of nanofluids at high solid loading, while simultaneously retaining electrochemical activity of nanoparticles. A scalable

single step procedure for the surface grafting of small organic molecules onto nickel (II) hydroxide nanoparticles ($Ni(OH)_2$) is demonstrated. Modified nickel hydroxide nanoparticles have a small amount (<3 wt%) of the grafting moiety on the surface, which helps formulating stable dispersions with up to 60 wt% of solid loading in alkali aqueous electrolytes with a maximum viscosity of 32 cP at room temperature. For comparison, suspension with 10 wt% of pristine nanoparticles shows viscosity of >2,500 cP. Suspensions of surface-modified $Ni(OH)_2$ particles also show up to 60% enhancements in thermal conductivity, as compared to base electrolytes. Electrochemical testing of the pristine and modified nanomaterials in the form of solid casted electrodes showed reversible discharge capacities exceeding 250 mAh/g, indicating comparable electrochemical activity of both samples close to the theoretical limit of 289 mAh/g.

A-7

Formation of Surface Oxides and Ag_2O Thin Films with Atomic Oxygen on Ag(111)

Derouin, Jonathan

Understanding the interaction of oxygen with transition metal surfaces is important in many areas including corrosion and catalysis. The oxygen/silver system in particular has been studied extensively both experimentally and theoretically. Interest is driven largely by the role of silver in two widely used industrial reactions: the epoxidation of ethylene to produce ethylene oxide, and the partial oxidation of methanol to produce formaldehyde. In addition, the oxygen/silver system can serve as a model for the dissociative chemisorption of diatomic molecules on close packed metal surfaces. Despite extensive research, the oxygen/silver system is still not well understood. To better understand this system, we use UHV-STM, AES, LEED and TPD to study the adsorption of atomic O on an Ag(111) crystal. Atomic O is generated by thermally cracking molecular O. By varying the power of the thermal cracker we are able to change the flux of atomic O reaching the Ag surface. Using lower O fluxes, we have been able to produce large p(4x4), p(4x5√3), and c(3x5√3) domains. Higher atomic O fluxes produce thin oxide structures that desorb at significantly higher temperatures than structures produced with lower O fluxes. We then use UHV-STM to further characterize the various oxide structures produced.

A-8

Investigation of Lattice Displacement Dynamics and Nanocatalytic Activity of Gold

Sasikumar, K.[1], A. Ulvestad[2], J.W. Kim[2], R. Harder[3], E. Maxey[3], J.N. Clark[4,5], P. Mulvaney[6], B. Narayanan[1], S.A. Deshmukh[1], S.K.R.S Sankaranarayanan[1], N. Ferrier[7], T. Peterka[7], and O.G. Shpyrko[2]

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[2] Department of Physics, University of California-San Diego, La Jolla, CA 92093
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[4] Stanford PULSE Institute, SLAC National Accelerator Laboratory Menlo Park, CA 94025
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[6] School of Chemistry & Bio21 Institute, University of Melbourne, Parkville, VIC 3010, Australia
[7] Mathematics and Computer Science Division, Argonne National Laboratory, Argonne, IL 60439

Multi-electron transfer processes are important areas of research for energy and biological applications. These processes require the use of favorable catalysts to achieve the fast kinetics rates necessary for practical purposes. Nanostructured catalysts offer promise in this regard, having shown improved activity and stability relative to their bulk counterparts. However, several theoretical challenges, such as understanding the strain and size dependent thermodynamics, and characterization challenges, such as imaging catalytic activity at the single particle level, still remain.

In this work, we use ascorbic acid decomposition facilitated by a gold nanoparticle as a model multi-electron transfer process to investigate the strain field evolution in the nanocrystal lattice during catalysis. Integrating ultrafast imaging with molecular dynamics (MD) modeling can provide crucial insights on the catalytic activity of gold in such processes.

Here, coherent x-ray diffractive imaging (CXDI) was used to observe reversible lattice distortions in gold nanocrystals upon exposure to ascorbic acid solutions. The lattice displacement dynamics are primarily concentrated on the surface of the gold nanoparticle during catalysis and are strongly size dependent. However, the magnitude of the observed effects is larger than predicted by electrowetting theory. A series of reactive MD simulations capture the reaction chemistry near the gold-acid interface more accurately and reveal an alternate paradigm for lattice dynamics, in addition to electrowetting theory.

A-9

Stabilizing Hybrid Perovskites against Moisture and Temperature via Non-Hydrolytic Atomic Layer Deposited Overlayers

Kim, In Soo[1,2] and Alex B.F. Martinson[1,2]

[1] Materials Science Division, Argonne National Laboratory, Argonne, IL 60439
[2] Argonne Northwestern Solar Research (ANSER) Center, Evanston, IL 60208

Organic-inorganic hybrid perovskites have emerged as one of the most promising materials classes for demanding optoelectronic applications that include photovoltaics, light emitting diodes, and photodetectors. For photovoltaic application in particular, an important prerequisite is the long-term stability against environmental moisture and temperature. Most hybrid perovskite materials are, however, prone to both moisture- and temperature-induced degradation, and will therefore require new and perhaps numerous stabilization strategies to retain their desirable properties. While atomic layer deposition (ALD) provides an efficient route to synthesizing pinhole-free barriers with chemical control, typical processes involving water as an oxygen source immediately trigger the decomposition process in hybrid perovskites. Here, we utilize a novel non-hydrolytic surface chemistry to synthesize ultrathin oxide barriers directly on hybrid perovskites without damage. Utilizing water-free ALD Al_2O_3 passivation, a minimum of tenfold increase in stability against relative humidity (RH) 85% was achieved along with a dramatically improved thermal resistance (up to 250°C). Moreover, we extend this approach to synthesize nh-TiO_2 directly on hybrid perovskites to establish its potential in inverted photovoltaic devices as a dual stabilizing and electron accepting layer, as evidenced by photoluminescence (PL) quenching.

A-10

Direct Synthesis of Hexagonal Boron Nitride Films and Their Heterostructures with Transition Metal Dichalcogenides

Behura, Sanjay, Phong Nguyen, Songwei Che, Rousan Debbarma, and Vikas Berry

Department of Chemical Engineering, University of Illinois at Chicago, IL 60607

Owing to ultra-smooth surface, nominal surface roughness scattering, and charged impurity scattering, the hexagonal boron nitride (h-BN) films can enhance the charge carrier transport in interfaced transition metal dichalcogenides (TMDs). All the present processes to design h-BN-based heterostructures involve transfer or exfoliation of at least one of the layers. Therefore, rational chemistries and process techniques are still required to produce large-area, transfer-free, directly grown TMDs/BN heterostructures. Here, we demonstrate a novel boron-oxygen chemistry route for oxide-assisted nucleation and growth of large-area,

uniform, and ultrathin h-BN directly on oxidized substrates (B/N atomic ratio = 1:1.16±0.03 and optical band gap = 5.51 eV). These intimately coupled, van der Waals heterostructures of MoS_2/h-BN and WS_2/h-BN get advantage from 6.27 folds reduced roughness of h-BN in comparison to SiO_2. This leads to reduction in surface roughness scattering and charged impurity scattering for the enhancement of intrinsic charge carrier mobility for TMD-based heterostructures, as verified by the increase in electrical conductivity (5 times for MoS_2/h-BN and 2 times for WS_2/h-BN). Further, the heterostructures are devoid of wrinkles and adsorbates, which is critical for 2D nanoelectronics. The versatile process can potentially be extrapolated to realize a variety of heterostructures with complex sandwiched 2D electronic circuitry.

A-11

Kolipaka, Karthika Lakshmi

No Abstract Submitted

A-12

Direct Formation of Monolayer Graphene on Si-Based Dielectrics

Nguyen, Phong[1], Sanjay Behura[1], Vikas Berry[1], and Mike Seacrist[2]

[1] Department of Chemical Engineering, University of Illinois at Chicago, IL
[2] SunEdison Semiconductor

Graphene—a one-atom-thick planar sheet of carbon atoms—possesses a distinct combination of properties including ultrahigh carrier-mobility, ultrafast photodetection, sensitivity, tunable spintronics, strong/tunable optical absorption, carrier controlled interband/optical-transition, and quantum interference. To incorporate it into the semiconductor industry, direct growth of wafer scale, high-quality, monolayer graphene on silicon-based dielectrics (SiO_2 and Si_3N_4) is desired for the next step towards graphene electronics. In this presentation, we demonstrate a robust low-pressure chemical vapor deposition (LPCVD) process to directly synthesize uniform and high-quality graphene on SiO_2 substrate or quartz by utilizing catalytic activity of thin evaporated copper (Cu) film. Here, precursor methane (CH_4) gas is diffused through Cu grain boundaries to the interface between Cu and selected Si-based dielectric, where it is catalytically dissociated into active carbon species at elevated temperature. Further, the optimization of the process parameters (SiO_2 surface chemistry, reaction time, temperature, CH_4/H_2 flow rate ratio, and cooling rate) is discussed to further understand the mechanism and growth rate of graphene on chosen dielectric. Material analyzing techniques such as scanning Raman spectroscopy, x-ray photoelectron spectroscopy (XPS), and selectrive area electron diffraction (SAED) are employed for graphene's structural characterization. The Raman D-peak, G-peak, and 2D-peak occur at characteristic ~1350 cm^{-1}, ~1600 cm^{-1}, ~2700 cm^{-1}, respectively. The I_D/I_G ratio (~0.1) corresponds to a graphene cyrstalline sp^2 domain size of 50 nm. The XPS shows the presence of C=C bonding at 284.5 eV, further confirming the formation of graphene. Moreover, SAED analysis shows a single hexagonal pattern, and a d-spacing of 2.44, which also indicates the possbile formation of monolayer graphene. The AFM measurement confirms the controllable thickness of graphene (1–5 nm) via different growth conditions. Furthermore, the electrical properties and optical property of the produced graphene is also be presented. Our patented method allows us to achieve high-quality wafer-sized graphene on a silicon-based insulating substrate without the need of graphene transfer.

A-13

Bio-Interfaced Wrinkling of Graphene Materials: Structure and Electrical Properties

Deng, Shikai[1], Enlai Gao[2], Yanlei Wang[2], Soumyo Sen[3], T. S. Sreeprasad[4], Sanjay Behura[1], Petr Král[3,5], Zhiping Xu[2], and Vikas Berry[1]

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Graphene interfaced with biological cells is an important system with applications in cell actuated sensors, cell-driven field-effect-transistors (FETs), cell-excretion based FETs, and cell electrochemical transponders. However, little is known about cell induced mechanical actuation (such as wrinkling) of graphene. For example, local π–orbital stretching, dipolar doping, and/or carrier puddling caused by wrinkles in graphene directly influence its electronic and phononic properties. Here, we show that bacterium's high surface energy, transportable volatile content and shrinkable microstructure can induce controlled and confined wrinkles on interfaced graphene sheets. The relaxation of pre-stretched bacterial cell in vacuum results in graphenic wrinkles to orient in the longitudinal direction to the strepto-bacillus cereus cells with a texture aspect-ratio of 0.125. Coarse-grained molecular dynamics (CGMD) simulations suggest that tension in graphene prompts wrinkle formation with wavelength of ~34 nm, consistent with the observed wavelength of 32.4–34.3 nm. The strain change and wrinkles formation processes were studied by CGMD simulations and Raman spectroscopy. Under vacuum, native bacteria and the bacteria covered with graphene (previously stretched) dehydrate and shrink (stress released) to the same level; however, graphene covered bacterium does not rehydrate at atmospheric pressure, while native bacteria springs to original state upon rehydration. We will (a) demonstrate directed electrophoresis of bacterial cells between electrodes for position-controlled 2D-wrinkle placement and (b) discuss the transport properties through wrinkled graphene. These graphenic bio-interfaced wrinkles can lead to novel nano/bio microelectromechanical systems with applications in electrical cell actuation, dehydration, sensing, restraining, retention, electro-microfluidics, and controlled delivery.

A-14

Panuganti, Harsha

No Abstract Submitted

A-15

Feasibility of Short Period 2G-HTS Based Undulator

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Undulators are the heart of the storage rings and free-electron laser-based light sources that actually produce high-brilliance hard x-ray radiations. NbTi-based superconductive undulators (SCUs) have been recently developed and demonstrated to reach higher on-axis peak fields and therefore higher brilliance when compared to the field values achieved with conventional hybrid undulators. However, NbTi has nearly reached the limits of its performance. In addition, cooling NbTi coils is an extremely challenging

task. Because of these problems, REBCO (RE = rare earth, barium copper oxide) second-generation (2G) high-temperature superconducting (HTS) tapes have been considered to be an alternative due to their high engineering current densities and larger temperature stability margin; they can thereby be operated at higher temperatures, which can greatly simplify the cryogenics. In this study, we discussed a design for building a next-generation prototype undulator and addressed some of the problems related to fabricating an undulator magnetic structure using REBCO thin film superconductors.

A-16

Kovi, Kiran Kumar

No Abstract Submitted

A-17

Operando Investigation of the Hydriding Phase Transformation in Single Palladium Nanocubes

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Phase transitions in reactive environments are crucially important in energy and information storage, catalysis, and sensors. However, establishing the causal link between structure and function is challenging for nanoparticles as ensemble measurements convolve intrinsic single particle properties with sample size and shape diversity. Here we study the hydriding phase transformation in individual palladium nanocubes under operando conditions using coherent x-ray diffractive imaging. We directly observe two-phase coexistence in the single particle diffraction data. The phase transformation initiates as an incoherent precipitate at a cube corner and then penetrates further into the particle. The strain distributions of the α and β phases are markedly different, indicating elastic, concentration, and surface effects all play a role. A phase field model is constructed to interpret the phase transformation. Our results provide a general framework for understanding phase transformations in individual nanocrystals under operating conditions in reactive environments while highlighting the utility and importance of single particle investigations to understand important systems.

A-18

Development of a Rechargeable Ca-Ion Battery

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Less expensive and higher energy density rechargeable batteries are needed for mass produced electric vehicles as well as storage for intermittent energy generation sources. One option is to use lithium as a metallic electrode, which has been explored for decades but still has yet to be commercialized for rechargeable batteries. Other metals can be explored, such as Mg or Ca, since they are inexpensive and may suffer less from the dendrite growth and interface stability issues of lithium. Based on a lower

potential versus the standard hydrogen electrode and less stable surface films, Ca should be the better choice. In order to develop such a battery, we first developed a cell to allow for flexible electrolyte choice for testing cathode materials. During the cell development process, we found that corrosion of the current collectors was dominating the electrochemical capacity. After redesigning our cell geometry to prevent corrosion, we started testing cathode materials and found one that had reversible behavior with a reasonable capacity and voltage. After proving that the cathode actually intercalates Ca via x-ray diffraction (XRD), energy dispersive x-ray spectroscopy (EDX) and x-ray absorption near-edge structure (XANES), we searched and found a compatible anode.

A-19

Kinetic Monte Carlo Simulations of Organo-Metallic Vapor Phase Epitaxy of GaN on Various Crystal Orientations

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Understanding how to grow GaN films of desired crystal orientations is essential to obtain optimal performance of GaN-based LEDs and high-power electronics. We use the kinetic Monte-Carlo software SPPARKS developed by Sandia National Lab to simulate the growth behavior on m- and c-planes of GaN at different temperatures and deposition rates. The transformation of the growth mode from 3D to layer-by-layer to step-flow is found for m-plane surfaces when the temperature increases or deposition rate decreases. In contrast, the region of layer-by-layer growth is limited for c-plane surfaces with the same conditions as m-plane. The growth on m-plane is anisotropic, while it is isotropic on c-plane. These simulation results are consistent with recent in situ x-ray experiments. We also calculate the relationship between island spacing and the growth rate during layer-by-layer growth on m-plane, which is consistent with nucleation theory. Simulations of two-time correlations during crystal growth, which could be measured with coherent x-ray techniques, indicate that these will reveal new aspects of the atomic dynamics. The simulation results help us to understand the growth behavior observed in experiments and give guidance on synthesis of high-quality GaN thin films.

A-20

Friction and Wear of Carbon Films Derived from Natural Gas

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One of the major technological barriers in using compressed natural gas as a fuel for transportation vehicles is that the friction and wear of sliding parts and components in compressors must be low. To overcome these deficiencies, we are developing catalytically active nano-composite coatings that are capable of extracting their own slick carbon-rich boundary films from the natural gas itself. Under rubbing action, catalytically active nano-composite coatings reduce hydrocarbon molecules of natural gas (such as methane, etc.) into the superlubricious carbon films on rubbing surface which in turn reduce wear. Tests have shown that uncoated steel surfaces wear out very quickly and hence will not be suitable for use in natural gas; while with the nano-composite coating on sliding surfaces, the wear is reduced by more than 3 orders of magnitude. Using Raman spectroscopy and other surface sensitive techniques, we are exploring the chemical nature of protective carbon films forming on rubbing surfaces in order to better understand the underlying mechanisms and hence further optimize their functionality. The results of this

work may lead to increased uses of natural gas for transportation and other applications where compressed natural gas is needed.

A-21

WEST: Novel Scalable Software for in Silico Discovery of Materials for Energy

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The emergence of petascale computational resources has provided the opportunity to perform quantum simulations of unprecedented size, yielding results that can complement experimental observations and that can lead to the discovery of new materials, designed using principles revealed by basic science. Density functional theory (DFT) is the predominant tool used in first principle simulations, but typical exchange and correlation functionals do not provide an electronic structure with a high enough level of accuracy. Hybrid density functionals and many-body perturbation theory (MBPT)-based corrections offer the required high level of accuracy but are computationally demanding for the larger systems of interest in simulating disorder, defects, interfaces or quantum confinement. Here we present WEST, an open source massively parallel code developed at Argonne and The University of Chicago within the Institute for Molecular Engineering (www.west-code.org), which leverages petascale resources to solve large-scale systems with high accuracy. The quasiparticle electronic structure of systems relevant for energy conversion processes are presented, and the parallel performance of the code is discussed.

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A-22

Real-Time Imaging with Atomic-Level Spatial Resolution of Silicon Oxidation

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The investigation of the initial stages of molecular oxygen adsorption on Si(111)-7×7 with real-time and real-space visualization will be discussed in this presentation. We will present the first results from a newly built supersonic molecular beam paired with a scanning probe microscope instrument. The system has a custom scanning probe microscope with its surface plane normal to the beam. This geometric arrangement allows us to perform real-time and real-space in situ experiments. The study consists of exploring the potential energy surface for molecular oxygen adsorption on Si(111)-7×7. The questions that are being addressed are fundamental for issues relating to semiconductor oxidation as well as being of direct relevance to semiconductor processing. The site-specific locations of molecular oxygen reactivity on Si(111)-7×7 surfaces are not clear and remain a topic of current discussion. Recent spectroscopic studies show that by controlling the molecular beam energy (E_k) one can activate different adsorption pathways for molecules on surfaces. However, the effect of collimated and energy-selected beams impacting the surface has not been observed in situ at the local molecular level until now. The results indicate that using supersonic beams in this matter may provide enhanced control of semiconductor oxidation chemistry.

A-23

Nonclassical Nucleation Mechanism in Molten Urea

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Nucleation is a ubiquitous process of paramount importance in nature and industry. The manufacturing of high purity crystals with controllable shapes is a major challenge in material science and drug design. Despite its paramount importance, many of its aspects remain unknown to us, mostly because of the transient nature and small size of the embryo nuclei. For their atomistic resolution, molecular dynamics simulations are an effective tool to obtain information on nucleation of inorganic and organic compounds. In order to characterize the nucleation of urea from its melt, we have recently applied molecular dynamics coupled with enhanced sampling techniques such as metadynamics [1, 2]. In order to promote the formation of a crystal in a reversible way and isolate all the possible urea polymorphs, we designed a new collective variable based on the concept of local order and local density. Via the application of the well-tempered version of metadynamics, we were able to promote the formation of urea nuclei at different temperatures, highlighting the presence of a new possible polymorph. The final nucleation mechanism was found to be different from what classical nucleation theory suggests, with the embryo nucleus composed of two simultaneous polymorphs.

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A-24

Beyond-DFT Electronic Structure for Heavy Atoms and Large Systems: Spin-Orbit Coupling and Surface Defect Calculations Using Many-Body Perturbation Theory

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While density functional theory (DFT) is widely used, it gives large errors for several properties, such as semiconductor band gaps. The GW approximation to the Dyson equation is a very successful method which begins with a DFT calculation and computes corrections based on many-body theory. GW calculations have traditionally been extremely challenging to perform for large systems, but newly developed algorithms and a high performance code developed by some of the authors, WEST, greatly improve the efficiency of GW calculations. Here, we present extensions and applications of the WEST code. First, spin-orbit coupling is included in calculations, so that solids and nanoparticles containing heavy elements such as gold and lead can be calculated with much better accuracy. Second, we use WEST to refine the simulation of a dangling bond on a hydrogen-passivated silicon surface. This system shows promise for quantum information applications, and it is also an intermediate step toward the fabrication of complex atomic-scale silicon devices.

A-25
First Principles Simulations of Organic Solar Cells

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Solar cell devices based upon organic electronics possess many advantages relative to traditional silicon photovoltaics, including potentially inexpensive manufacturing, band gaps which are tunable through chemical modification, and high optical absorption coefficients. Recent progress in generating improved polymers for organic solar cells has suggested that precise electronic energy level alignment between multiple donor polymers (PTB7, PID2, etc.) significantly improves device performance. The effect of specific morphologies on device efficiency is difficult to determine experimentally, but our theoretical models can directly probe how structural changes affect electronic properties, such as band locations and band gaps. Using periodic plane wave DFT and many body perturbation theory (G0W0) calculations, we calculated the dependence of electronic states on order parameters such as backbone dihedrals. Hybrid density functional theory, in particular, performs well for these systems. Our results suggest that accurate description of the device performance must include a description of local disorder. In particular, the potential energy scans we performed suggest multiple possible configurations which differ significantly in electronic structure. Using the lowest energy conformations, our alignment of electronic energy levels is in good agreement with experimental values.

A-26
Particle Irradiation and Superconductors

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Disorder has complex effects on superconductivity: increasing the maximum current it carries while strongly affecting the properties of new high-temperature superconductors, but not those of standard s-wave superconductivity. Other electronic phases competing with superconductivity can also be affected by disorder thus promoting superconductivity. Introducing defects into a superconductor is therefore both an interesting tool for basic science studies and an active field of research for industrial applications. Here I will show that particle irradiations can markedly enhance the in-field critical current in commercial second-generation superconducting tapes [1]. Recently, using numerical simulations we optimized irradiation damage, and then demonstrated that oxygen irradiation can double the in-field critical of production line tapes in one second thus leading to a viable reel-to-reel manufacturing post-processing. In collaboration with theoreticians specialized in large-scale Ginzburg-Landau simulations of vortex dynamics, we investigated the optimal dose for maximum J_c at a given temperature and field, and the optimal mix of defects to reduce the anisotropy of J_c. Finally, we investigated the s+- order parameter in Fe-based superconductors [2] and the balance between superconductivity and charge order in 1/8 doped cuprates, using radiation-induced disorder and synchrotron x-ray diffraction in extreme environments.

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A-27

First Principles Analysis of Defect Thermodynamics and Ion Transport in Inorganic SEI Compounds: LiF and NaF

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The formation mechanism and composition of the solid electrolyte interphase (SEI) in lithium ion batteries has been widely explored. However, there is still relatively little known about the function of the SEI as a transport medium. Such critical information is directly relevant to battery rate performance, power loss, and capacity drop. Here, we report the results of first principles calculations on the defect thermodynamics, the dominant diffusion carriers, and the diffusion pathways associated with crystalline LiF and NaF, which are stable components of the SEI in Li-ion and Na-ion batteries. The thermodynamics of common point defects are computed, and the dominant diffusion carriers are determined over a voltage range corresponding to conditions relevant to both anode and cathode SEIs. Ionic conductivities are calculated as a function of voltage, considering the diffusion carrier concentration and the diffusion barriers as determined by Nudged Elastic Band calculations. Our analyses reveal that in both compounds, as compared other common inorganic SEI compounds such as Li_2CO_3 and Li_2O, the ionic conductivity is at least three orders of magnitude lower. The results quantify the extent to which fluorides pose rate limitations in Li and Na batteries.

A-28

Developing Protein Fibers into a Novel Technology to Meet Society's Needs

Solomon, Lee

Today's energy demands are quickly growing and the methods we use to meet them are harmful to the environment and not sustainable. Natural proteins generate and transport energy cleanly and effectively but have not been exploited for our needs due to their inherent complexity and specificity. Nanotechnology does not have these limitations but lacks the malleability of biological systems. Growing out from the interface of biology and nanotechnology are peptide amphiphiles (PAs): short proteins with a hydrophobic tail. These proteins form into long fibers if treated with base, and when polymerized are able to bind natural cofactors used in natural light harvesting and energy storing processes. Compared to modern industrial materials that harvest and transfer solar energy or transmit electricity, PA assemblies provide more control, adaptability, and industrial scalability, as they can be grown in bacteria. Additionally, the harsh conditions needed to make common metal components can be avoided leading to environmentally friendly wires. I am currently reengineering these proteins to incorporate new functions. First, I am attaching the fibers to electrodes and having them transmit electricity. PAs are also being designed to harvest, transfer solar energy and drive light-powered machines. Finally, I am designing the fibers to assemble into specified patterns that incorporate multiple cofactors and peptide sequences to generate complex functions not currently possible, such as micro-sensors and environmentally responsive switches. The work presented here will elevate PA fibers to a new level that will directly benefit society.

A-29

Quantifying Protein-Protein Binding Energy and Entropy Using Molecular Dynamics Simulations

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Protein-protein interactions (PPIs) represent a critical aspect of a wide range of biological processes, as most proteins need to associate to various binding partners to carry out their functions. While the basic principles of PPIs are generally understood, it is a grand challenge to accurately predict the binding affinity quantitatively for any given complex. Recently, this potential of mean force (PMF)-based methodology was extended to a much larger protein-peptide sys- tem, and we accurately determined the absolute binding free energy between the receptor protein and the ligand peptide. We plan to employ our PMF-based methodology to probe effects of mutations in thermodynamics of protein-protein interaction. Furthermore, thermodynamic decomposition of barstar-barnase protein complex association is attempted to quantify not only to probe the effect of mutation on binding free energy but also on binding entropy.

A-30

Predicting the Pressure-Dependent Kinetics of Radical-Radical Reactions: A Priori Solution of the Two-Dimensional Master Equation

Verdicchio, Marco[1], Ahren W. Jasper[2], Kenley M. Pelzer[1], Yuri Georgievskii[1], Michael P. Burke[3], James A. Miller[1], and Stephen J. Klippenstein[1]

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The description of the pressure dependence of radical-radical reactions is a key point for the kinetic modeling of combustion and atmospheric processes. The ability to predict pressure-dependent rate parameters for such reactions would dramatically improve the utility of theoretical kinetics simulations for the modeling of practical chemical problems, especially for extreme conditions where the validity of experimental results is questionable. To address this problem, Jasper et al. [1] proposed a new full a priori two-dimensional master equation (2DME) scheme. This approach uses trajectory simulations to predict the collision-induced transitions in the energy, E, and angular momentum, J, thereby overcoming the empiricism and consequent uncertainties arising from the formulation of collisional energy transfer parameters adopted in prior theoretical kinetics studies. In the present work, we have coupled this scheme with multireference electronic structure based transition state theory methods to calculate the pressure-dependent rate constant for the reaction of hydrogen with molecular oxygen in different bath gases. This is perhaps the single most important pressure-dependent reaction in combustion and is also of significance

to atmospheric chemistry. The effect of the predicted rate constant on combustion is explored through flame speed simulations for the H_2/O_2 system under a variety of conditions.

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A-31
Coordination Chemistry of Isostructural Actinide and Lanthanide Thiocyanates

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Thiocyanate and other soft-donor ligands have long been known to enhance separation of trivalent lanthanides and actinides. However, the origin of this enhanced separation remains unknown. Our recent work revealed a series of isostructural complexes common to both the lanthanides and actinides providing a unique opportunity to study periodic trends among thiocyanate complexes of the f-elements. A combination of crystallographic, vibrational, and optical spectroscopy was used to obtain new insight into the nature of the M-NCS bond. These data suggest little covalent overlap with the thiocyanate π-system but a strong correlation between the Lewis Acidity of the metal and the M-NCS bond strength.

A-32
Comparisons of Thorium Nitrate and Thorium Sulfate Hydrolysis Products

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Hydrolysis and condensation reactions play an important role in the aqueous chemistry of metal ions with high charge density under all but very acidic solution conditions. Motivated by a desire to understand their solution speciation and corresponding structural motifs of resulting precipitates, we have focused on the hydrolysis, condensation, and complexation of tetravalent actinide ions. Nitrate and sulfate anions have been used to isolate condensed Th oligomers, with very different results. Solid products isolated from nitrate solutions within a wide pH range reveal no oxo/hydroxo connectivity but instead they all contain monomeric thorium species. In contrast, in the presence of sulfate, a complex thorium sulfate hydrate cluster $Th_3[Th_6(OH)_4O_4(H_2O)_6](SO_4)_{12}(H_2O)_{13} \cdot 8H_2O$ with a $[Th_6(OH)_4O_4(H_2O)_6]^{12+}$ hexanuclear core has been isolated. These different condensation behaviors can be partially attributed to the different coordination modes of the two anions with Th^{IV} ions. Nitrate chelates with Th^{IV} exclusively in a terminal-bidentate mode, even in solution, while sulfate is able to bridge Th^{IV} centers, enabling the formation of polynuclear structures.

A-33
Elucidating the Flame Chemistry of Common Combustion Radicals

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Radical populations in flames are responsible for driving combustion, whether through fuel break-down (via abstraction reactions and unimolecular decompositions), regulating chain branching vs termination reactions, or providing heat release. As such, accurately describing the kinetics of these radicals is

essential for the development of predictive combustion kinetics model. In this work, we have explored the high temperature kinetics of several key combustion radicals. First, we have characterized the effect of including radical + fuel-radical well-skipping reactions in low-pressure laminar flame simulations and shown their effect on speciation predictions. Secondly, we have utilized theory and modeling to simulate isotopic methanol experiments to, for the first time, establish the role of $CH_2OH \rightarrow CH_3O$ isomerization, and subsequently the direct decompositions of these two radicals. Lastly, we have determined that all weakly-bound combustion radicals (bond energies < 50 kcal/mol) have some tendency to undergo direct decomposition as a result of the dissociation process interfering with the internal energy relaxation process. In particular, we have characterized this effect for the formyl radical, HCO, and simulations indicate that direct decomposition of this radical impacts flame propagation in most hydrocarbon/oxygenated fuels.

A-34

Parameterized Quantum Chemistry Methods for High-Performance Computing

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Parameterized quantum chemistry (PQC) methods, such as semi-empirical molecular orbital (SEMO) methods, or density functional based tight-binding (DFTB) methods, offer a computational cost and accuracy in between molecular mechanics and ab initio methods. We present our efforts on increasing the accuracy and reducing the computational cost of PQC methods. For the former, we performed high- accuracy quantum chemistry calculations (e.g., coupled cluster calculations at the basis-set limit) for transition metal oxide clusters to extend the training data for these systems. For the latter, we attacked the computational bottleneck in PQC calculations, which is the matrix diagonalization step, and developed the Shift-and-Invert Parallel Spectral Transformations (SIPs) method. SIPs decomposes the eigenvalue spectrum into slices and independently processes each slice to find its eigensolutions in parallel. We demonstrated the capabilities of SIPs using DFTB applications on metallic single-wall carbon nanotubes, diamond nanowires, and crystal diamonds of varying sizes and demonstrated the strong scaling of SIPs by utilizing more than 200k cores on BG/Q supercomputer, Mira. We recently integrated SIPs into a quantum chemistry code, QETSc, which can perform SEMO type calculations. We analyze the performance of QETSc for different stages of a self-consistent-field calculation.

A-35

From Molecular Coordination to Mesoscopic Structures of Solvent Extraction Solutions: Multiscale Experimental and Theoretical Studies

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With the great environmental and economic challenges of this century, it is of great importance to enhance and/or develop new processes for a better management of strategic resources, such as rare earth elements or uranium and plutonium from used nuclear fuel. Solvent extraction technology is the foundation of most processes for metal separation. Understanding the fine chemistry of those complex processes is the key for more efficient designs. Different chemical systems currently used in solvent

extraction processes of importance, such as malonamide organic extractants, were investigated in order to get a better understanding of the chemistry involved, both at a molecular scale (coordination chemistry) and at the mesoscale (aggregation). A study combining molecular coordination, supramolecular structure speciation, and molecular dynamic simulations has been performed through the analysis of data from multiple characterization techniques like small-angle x-ray scattering (SAXS) and extended x-ray absorption fine structure spectroscopy (EXAFS). Correlation of molecular dynamic simulations results with experimental data has given new insights not only into the structural organization of organic phases and the interactions responsible for the formation of such structures but also into the coordination of both the metal ion and counter-ion in organic media, which explain particular physicochemical behaviors of these organic solutions. This new approach could be generalized to other solvent extraction systems and lead to a better design of solvent extraction processes, which is of primary need for the refining of some elements or for recycling the used nuclear fuel.

A-36

Shining Light on Molecules: Membrane/Peptide Study Highlights the Utility of a Diverse Experimental Toolbox

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As modern science becomes increasingly interdisciplinary, cutting-edge studies commonly require a multitude of experimental and theoretical tools. This presents an overview of complementary techniques including 2DIR spectroscopy, vibrational sum frequency generation (VSFG) spectroscopy, and fluorescence microscopy. 2DIR probes equilibrium kinetics and dynamics on femtosecond to picosecond time scales. VSFG signal only arises from samples without inversion symmetry, making it an interface-specific vibrational spectroscopy; researchers use VSFG to probe interfacial chemical structure—systems traditionally difficult to access. A multifaceted approach is used to study the pH-driven pore-penetrating peptide GALA. GALA was designed to mimic viral infusion proteins and continues to draw interest as a possible addition to nanoparticle therapeutics to trigger endosomal escape after cellular internalization. Real-time imaging of surface-tethered giant unilamellar vesicles shows that the lipid bilayer radius-of-curvature has a negligible effect on GALA-induced leakage kinetics. SFG spectroscopy and surface pressure measurements reveal that GALA remains active after incorporation into the membrane and can be reversibly switched between its active and inactive states even after incorporation into a lipid membrane.

A-37

An Experimental and Theoretical Study of the Thermal Dissociation of Phenylchloride

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The thermal decomposition of halo-benzene species is an important reaction in waste material incineration, and has recently been shown to provide a convenient experimental source of *o*-benzyne and phenyl radicals. The chemistry of both *o*-benzyne and phenyl radicals are significant in the formation of

polycyclic aromatic hydrocarbons (PAH) and soot. In order to successfully model the formation of soot in combustion environments the rates of the pertinent reactions involved must be accurately quantified. Shock tubes provide a useful means of investigating chemistry under conditions relevant to combustion. In this work, the dissociation of phenylchloride, dilute in krypton, has been studied over a broad range of temperatures (1760–2520 K) and pressures (30–421 Torr) in a diaphragmless shock tube (DFST), using laser Schlieren (LS) densitometry to measure axial density gradients behind the incident shock wave. The resulting experimental density gradients are dependent on both the kinetics and heats of the reactions occurring, and therefore provide information on both the rates, and on the specific chemistry involved. All 83 experimental density gradients can be successfully simulated using a model consisting of 23 reactions. The results presented here are consistent with initial dissociation of phenylchloride proceeding via two channels, resulting in formation of phenyl radical + Cl, through C – Cl bond fission, or benzyne radical + HCl, via a roaming path; the rates of each channel associated with the initial decomposition of phenylchloride have been corroborated by theory. Secondary reactions between the parent phenylchloride and radical products provide an additional source of *o*-benzyne and phenyl radicals to the system. Both dissociation and self-reactions of *o*-benzyne and phenyl radicals are required by the model to satisfactorily simulate the experimental density gradients.

A-38

Ab Initio Kinetics for the Decomposition of Unsymmetrical Di-methylhydrazine $(CH_3)_2NNH_2$

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A key feature of hydrazines is that they contain weak N-N bonds and any C-N bonds are only slightly stronger. These simple bond fissions produce two radicals that interact generally through strong dipole-dipole interactions and hydrogen bonding interactions. As a result, the potential energy surface (PES) for the interactions between the two incipient radicals is remarkably complex showing multiple minima and multiple pathways to a variety of products. We present a detailed exploration of the PES for UDMH on the basis of high level ab initio calculations. For illustrative purposes we have generated a set of planetary plots, which highlight the topography of the long-range interactions, for a range of N-N and C-N fragment separations. Analytic representations of the interactions for the N-N and C-N fissions are obtained via fits to $\sim 10^5$ CASPT2(2,2)/avdz ab initio data points. These analytic surfaces are utilized in rigid body dynamics (RBD) simulations of the branching between simple bond fission and other roaming related channels involving various H abstractions. Finally, utilizing the results of these RBD calculations and ab initio calculations, the master equation (ME) is solved, obtaining high-level predictions for the full set of thermal rate coefficients over a range of temperatures and pressures.

A-39

Experimental Investigation of the Pyrolysis of Cyclopentane

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Cycloalkanes make up a significant portion of conventional liquid fuels, including diesel, jet fuel, and gasoline, and yet have not been as extensively studied as straight-chained and branched alkanes. Furthermore, liquid fuels derived from oil sands and shale contain a higher proportion of cycloalkanes compared to well-oil. Here, the pyrolysis of cyclopentane was studied under combustion-relevant conditions using laser schlieren in a diaphragmless shock tube at 1500–2100 K. The diaphragmless shock tube is a powerful tool in studying combustion-relevant systems because it provides a means to heat a sample to combustion temperatures effectively instantaneously, while providing excellent control over both temperature and pressure. Laser schlieren provides information on the rates of reaction and heats of reaction for the chemistry taking place after the rapid rise in temperature. Development of a kinetics model used to simulate the experiments is also presented. Pyrolysis of cyclopentane (C_5H_{10}) takes place primarily through a ring-opening isomerization to 1-pentene, which in turn immediately dissociates to allyl (C_3H_5) and ethyl (C_2H_5) radicals. The resulting radicals then drive secondary chemistry, by which cyclopentane is lost via hydrogen abstraction to cyclopentyl radicals (C_5H_9). Comparisons to other cycloalkanes, such as cyclohexane and dioxane, are also made.

A-40

Process Scale-up: In Situ Biogas Upgrading during Anaerobic Digestion of Food Waste Amended with Walnut Shell Biochar

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With large volumes of organic municipal solid waste produced in the US each year (78.7 million tons) there is potential to develop a viable biogas industry via anaerobic digestion (AD) that can boost the economy and provide a reliable, distributed source of renewable energy while reducing greenhouse gas emissions. Biogas from AD of food waste consists mainly of methane (CH_4), carbon dioxide (CO_2) which can be upgraded for utilization in combined heat and power systems, as renewable natural gas or as a vehicle fuel. Some of the main barriers to commercialization of an AD industry include highly variable organic waste characteristics and volume, process economics, and biogas clean up requirements. This process overcomes these barriers by evaluating a low-cost in situ CO_2 removal process during the AD of food waste with walnut shell biochar, a waste carbonaceous solid produced from gasification or pyrolysis. The biochar has favorable characteristics with a high surface area (110 m^2/g), high ash content (43.2% dry weight), and high concentrations of calcium and magnesium (31% CaO and 8.4% MgO of the ash content, respectively), allowing for efficient CO_2 removal. The AD process was scaled up from 0.5 L batch reactors to 14 L 2-stage semi-continuous reactors while maintaining a high methane content (>80% CH_4) resulting from 40–70% CO_2 removal. Biochar addition increased alkalinity and pH, providing sustainable process stability for thermophilic AD despite the high variability of the food waste. The increased methane content will allow for more efficient biogas upgrading, improving process economics.

A-41

Performance Enhancement of an Internal Combustion Engine CFD Simulation on IBM BG/Q

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An internal combustion (IC) engine computational fluid dynamics (CFD) simulation was scaled on up to 4,096 processors on Mira and an IBM BG/Q supercomputer. The simulation was performed using CONVERGE, commercial CFD software for IC engine simulation. Performance optimization was focused in the near-ignition portion of the simulation, which is typically the most computationally intensive owing to small timescales associated with calculating chemical kinetics in every CFD cell. First, I/O was optimized in terms of reading restart files, as well as writing restart files and outputs for post-processing. The code was modified so that only one rank would read all the restart data and then broadcast to other ranks with caching on the local compute node. This resulted in restarting time (for a 4 GB restart file) reduction from 2 hours to 5 minutes. Further, writing operations were sped up using MPI I/O, resulting in a writing rate going up from 400 seconds/GB to 1–2 seconds/GB. A novel load balancing scheme for chemistry calculations was developed and implemented in the code, wherein cells are distributed to ranks for chemistry solution, with a weighting factor based on the chemistry penalty in each cell from the previous time step. This resulted in an 8-times improvement in load balance and a 3.4-times faster time to solution. With this improved scheme, we achieved a scaling efficiency of 93% on 2,048 cores and of 80% on 4,096 cores of Mira.

A-42

Electromechanically Controlled Flat Optical Devices

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Recently, flat optical elements, like lenses and beam deflectors, have come to the forefront of ongoing scientific research. These devices, often referred to as “metasurfaces,” use sub-wavelength dimension plasmonic or dielectric resonators, arbitrarily spaced on a two-dimensional (2D) plane, to mimic the phase profile of any conventional bulk optical device and beyond. However, these nanostructured 2D devices have so far been passive. In this work, we introduce a useful concept of actively controlling these flat optical devices. We present a prototype: an electromechanically controlled flat lens that focuses in the mid infrared part of the spectrum. The lens is fabricated on a 2-µm thin membrane following standard photolithography processes and integrated with a microelectromechanical system (MEMS) device. The MEMS platform can control the tilt angle of the lens by electrostatic actuation. Such electromechanically controlled, metasurface-based flat devices are compact and lightweight compared to their conventional bulky counterparts. Such devices promise to provide faster, more efficient, and often enhanced functionalities.

A-43

Large-Eddy Simulations of Engine Spray and Flow Variability in Direct-Injection Spark-Ignition Engines

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The use of direct-injection in spark-ignition (DISI) engines has large theoretical benefits to engine efficiency and emissions, but real gains have been limited by cycle-to-cycle variations (CCVs). Computational fluid dynamics (CFD) simulations could help understand the sources of engine CCVs, and potential methods to reduce them and gain more of the theoretical benefits of DISI operation. Traditional Reynolds-averaged Navier-Stokes (RANS) CFD simulations are not able to capture these CCVs well, but more recent large-eddy simulation (LES) methods use a different averaging approach and provide a promising method to capture and explore CCVs in CFD simulations. The presented work demonstrates the ability of LES to capture CCVs in a motored DISI engine. Variability in fuel spray events is more difficult to capture because the variability is due to processes that are not directly modeled in typical engine simulations, but instead appear as part of simulation boundary conditions. Two methods to incorporate spray variability into simulations are also presented.

A-44

Numerical Modeling of the Lake Mary Road Bridge for Foundation Reuse Assessment

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The project uses numerical techniques to assess the structural integrity and capacity of the bridge foundations and, as a result, reduces the risk associated with reusing the same foundation for a new superstructure. Lake Mary Road Bridge located southeast of Flagstaff, AZ, was chosen for testing. Data gathered during nondestructive tests performed on-site were used to build numerical models and run computational analyses on a high-performance computer cluster with a goal to assess the structural integrity of the bridge and foundations, including the suitability of the foundation for reuse, and assess what nondestructive tests to perform on-site and what type of monitoring to use after construction. Extensive numerical modeling was done to determine the response of the superstructure, foundations, and bedrock to existing loads. It was shown that the developed numerical model can be used to simulate a range of different nondestructive tests. Static, dynamic, and impulse loading cases were considered. The model predictions of structural behavior under various loads appear to be as accurate as the physical measurements.

A-45

Modeling of Internal Nozzle and Spray Formation of Gasoline Direct Injection Engines in Eulerian Framework

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The present work involves modeling internal and near-nozzle flows of a gasoline direct injection (GDI) nozzle utilizing HPC resources at Argonne. The ECN Spray G conditions have been considered for these simulations. The nominal geometry of the Spray G injector has been used for these simulations. Best practices for numerical simulation of the two-phase flow evolution inside and the near-nozzle regions of the Spray G injector are presented. The mass flow rate prediction was in reasonable agreement with experimental data for a specific and only available condition. The capability of assessing the influence of different thermodynamic conditions on the two-phase flow nature has been established, by predicting nonflashing, moderate flashing, and intense flashing and correlating with the degree of superheat and nondimensional numbers, such as the Jakob number. Mild vapor formation inside the holes of the injector was predicted for flashing and nonflashing conditions, suggesting sufficient depressurization of liquid fuel in a GDI nozzle. The outlet domain size has been observed to be of critical essence to avoid numerical errors occurring due to the reflective boundary condition. The possibility of plume-to-plume interaction has been predicted under intense flashing conditions with the help of the current study. Hole-to-hole variations in mass flow rates were predicted.

A-46

Producing Pipeline-Quality Biomethane via Anaerobic Digestion of Sludge Amended with Corn Stover Biochar with In Situ CO_2 Removal

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This study presents a novel process for producing pipeline-quality biomethane by anaerobic digestion (AD) of sludge with in situ biogas cleanup and upgrading using corn stover biochar. The biochar has high surface area (105 m^2/g), high ash content (45.2% dry weight), and high concentrations of potassium, calcium, and magnesium (14.2% K_2O, 3.9% CaO, and 4.2% MgO) of the ash content. The biochar-amended digesters produced near-pipeline-quality biomethane (>90% CH_4 and <5 ppb H_2S), facilitated CO_2 removal by up to 86.3%, boosted average CH_4 content in biogas by up to 42.4% compared to the control digester, close to fungibility of natural gas. The biochar addition enhanced the methane yield, biomethanation rate constant, and maximum methane production rate by up to 7.0%, 8.1%, and 27.6%, respectively. The biochar addition also increased alkalinity and mitigated ammonia inhibition, providing sustainable process stability for thermophilic sludge AD. The biochar-amended digestate is enriched with nutrients such as potassium, nitrogen and phosphorus, and therefore has great potential for soil applications.

A-47

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This poster describes an analysis of a variable speed heat pump (VSHP), which responds to direct load control (DLC) signals to provide grid frequency regulation (GFR) ancillary service, while ensuring the comfort of building occupants. A data-driven dynamic model of the VSHP is developed through real-time experimental studies with a time horizon ranging from seconds to hours. The model is simple, yet still sufficiently comprehensive to analyze the operational characteristics of the VSHP. The DLC scheme is then experimentally applied to the VSHP to evaluate its demand response (DR) capability. Two control methods are considered for a practical implementation of the DLC-enabled VSHP and a further improvement of the DR capability, respectively. Additionally, a small-signal analysis is carried out using the aggregated dynamic response of a number of DLC-enabled VSHPs to analyze their contribution to GFR in an isolated power grid. For experimental case studies, a laboratory-scale microgrid is then implemented with generator and load emulators. We show that the DLC-enabled VSHP can effectively reduce grid frequency deviations and required reserve capacities of generators.

A-48

Synthesis of Layered-Layered Cathode Materials Using a Taylor Vortex Reactor

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Advances in lithium ion battery (LIB) materials are led by the development of new synthesis methods where the production of materials in a scalable and continuous route is often critical when the process development moves to large scale quantities. In a LIB, one of the most performance-limiting components is the cathode, which also limits the overall performance of the battery. Among the other synthesis methods, co-precipitation from aqueous processes is known to yield the best cation mixing within the structure, in particular for the synthesis of cathode precursors for batteries. Batch and continuous stirred tank reactors (CSTRs) are by far the most widely used systems used in the battery industry, yet have low reproducibility, product efficiency, and undergo very long stabilization times due to low mass transfer rate. In this study, we propose to enhance the cathode precursor particle features (e.g., morphology, high crystallinity and density) using an advanced micro-mixing reactor, Taylor vortex reactor (TVR). This is a new emerging synthesis technology using its strong agitation capability by Taylor vortex flow to continuously prepare highly crystalline, size-tunable and spherical precursor particles in a relatively short time (by 3 times) compared to the conventional CSTR.

A-49

Modeling Reacting Spray Flames Using Large Eddy Simulation

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In this study, LES of n-dodecane spray flame is performed using a detailed combustion model along with a dynamic structure subgrid model. A high-fidelity resolution mesh is employed with a cell size of 0.0625 mm in the entire spray and combustion regions. The liquid spray is treated with a traditional Lagrangian method and the gas-phase reaction is modeled using a detailed combustion model consisting of 103 species. LES solution is observed to have multiple ignition spots in the mixing layer simultaneously while the main ignition initiates in a clearly asymmetric fashion. Transient flame development and soot predictions by LES presents good agreement with experiments. Multiple LES realizations were performed to understand the variation among realizations and to establish a methodology to compute statistical averages of relevant quantities. A relevance index analysis shows that 5 realizations are enough to obtain 99% similarity in the major statistically averaged quantities, if an azimuthal averaging is performed over 35 planes. The different LES realizations are performed by two ways—perturbing the spray breakup model parameters and perturbing the initial turbulence intensity in the computational domain. It is shown that both these methods lead to similar realization-to-realization variability in the flame structure.

A-50

A Multiscale Approach to a Class of Semidefinite Programs

Lin, Fu, Zichao Di, and Sven Leyffer

We consider a multiscale approach to a class of semidefinite programs that arises from combinatorial optimization problems on graphs. Our multiscale approach produces a sequence of progressively coarser problems by coarsening the underlying graphs. We use the solution of each coarse problem to provide an initial approximation to the solution at the finer level. At the coarsest level we employ Newton‘s method for high accuracy solutions, and at finer levels we take advantage of the inexpensive coordinate descent scheme. We show the competitiveness of our hybrid multiscale approach by comparing with SDPT3 over synthetic graphs and real-world power networks up to 5,000 buses.

A-51

Scaling Geometric Multigrid Preconditioners for DPG Systems

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The discontinuous Petrov-Galerkin finite element methodology of Demkowicz and Gopalakrishnan (DPG) [1] allows computation of solutions that minimize the residual in a user-controllable energy norm and includes a mechanism for measuring the error in that norm. Moreover, the method is stable even on coarse meshes, allowing automatic adaptivity starting from a coarse mesh. Camellia [3] is a C++ framework for rapid development of DPG solvers. To date, the iterative solvers available to Camellia have used “off-the-shelf“ preconditioners from Trilinos [2], which performed poorly in the context of adaptivity; thus, we employed direct solvers in previous work. The consequent limitation on the scalability of our computations motivates the present work—developing preconditioners for DPG

systems. In Camellia, we are interested in algorithms that support a wide range of PDE applications. Therefore, we seek a preconditioning strategy that, as far as possible, can be determined at runtime based on features of the PDE. For Camellia solves, we have rich geometric information in the form of the hierarchically refined mesh. This has led us to experiment with geometric h- and p-multigrid preconditioners with Schwarz smoothers for DPG problems. In this poster, we report our results to date, which are promising.

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A-52

Tell Me What Do You See: Detecting and Summarizing Perceptually Separable Patterns for Exploratory Data Analysis

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Data visualization leverages the capacity of the human visual perceptual system to see trends and spot outliers in the data. Overview displays can quickly highlight such features, but it is often infeasible to design a single display that conveys all the relationships of interest in a large information space. Navigation techniques, such as pan-and-zoom, can help by showing focused projections that depict subsets of the data at a time. However, viewers may not have the time or the cognitive bandwidth needed to attend to all relevant projections, causing them to potentially miss important structures in the data. Inspired by the way visual perception works, we present a method for semi-automated analysis of visualizations to aid users in exploratory analysis. The technique makes minimal assumptions about data types but leverages user's intuition on what is interesting in the data. Users start by specifying visual mappings in which they are interested. The computer then traverses the data, characterizing how these visual mappings "change" as it navigates the data space. The computer then presents a visual/verbal summary of the salient patterns it found in the data. This technique can significantly reduce the amount of time users spend analyzing visualizations. Additionally, it can be optimized to guarantee that users get an equitable coverage of all the prominent patterns in their data.

A-53

Data Acquisition with GPUs for the Muon *g*-2 Experiment at Fermilab

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A new measurement of the anomalous magnetic moment of the muon, $a_\mu \equiv (g-2)/2$, will be performed at the Fermi National Accelerator Laboratory. The most recent measurement, performed at Brookhaven National Laboratory and completed in 2001, shows a 3.3–3.6 standard deviation discrepancy with the standard model value of *g*-2. The new measurement will accumulate 20 times those statistics, measuring *g*-2 to 140 ppb and improving the uncertainty by a factor of 4 over that of the previous measurement. The data acquisition system for this experiment must have the ability to create deadtime-free records from

700 μs muon spills at a raw data rate of 18 GB per second. Data will be collected using 1,296 channels of TμTCA-based 800-MSPS, 12-bit waveform digitizers and processed in a layered array of networked commodity processors with 24 GPUs working in parallel to perform a fast recording of the muon decays during the spill. The system will be controlled using the MIDAS data acquisition software package. The described data acquisition system is currently being constructed and will be fully operational before the start of the experiment in 2017.

A-54

Skin Temperature Recovery Rate as a Potential Predictor for Radiation-Induced Skin Reactions

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The goal was to assess the potential of dynamic infrared (IR) imaging to evaluate early skin reactions during radiation therapy in cancer patients. Thermal images were captured by our homebuilt system consisting of two flash lamps and an IR camera. The surface temperature of the object was first raised by ~ 6°C from ~1-ms flashes; the camera then captured a series of IR images for 10 seconds. For each image series, a basal temperature was recorded for 0.5 second before the flash was triggered. The temperature gradients (ε) were calculated between a reference point (immediately after the flash) and at time points of 2, 4, and 9 seconds after that. A 1.0-cm region of interest (ROI) on the skin was drawn; the mean and standard deviations of the ROIs were calculated. The standard ε values for normal human skins were evaluated by imaging three healthy subjects with different skin colors. All of them were imaged on three separate days for consistency checks. The temperature gradient, which is the temperature recovery rate, depends on the thermal properties of underlying tissue. The average ε values for three volunteers averaged over three measurements were 0.64±0.1, 0.72±0.2 and 0.80±0.3 at 2, 4, and 9 seconds, respectively. The standard deviations were within 1.5–3.2%. One of the volunteers had a prior small skin burn on the left wrist and the ε values for the burned site were around 9% (at 4 seconds) and 13% (at 9 seconds) lower than that from the nearby normal skin. In conclusion, the temperature gradients from the healthy subjects were reproducible within 1.5–3.2 % and that from burned skin showed a significant difference (9–13%) from the normal skin. We have an IRB-approved protocol to image head and neck patients scheduled for radiation therapy.

A-55

Tau Neutrino Contamination in the Energy Spectrum of the NO*ν*A Experiment

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We are presenting an analysis to estimate the tau neutrino background in the far detector energy spectrum of the NuMI Off-Axis ν_e Appearance (NOνA) experiment [1]. The NOνA experiment is a currently active, long-baseline neutrino oscillation experiment designed to study $\nu_\mu \rightarrow \nu_e$, $\bar{\nu}_\mu \rightarrow \bar{\nu}_e$, $\nu_\mu \rightarrow \nu_\mu$, $\bar{\nu}_\mu \rightarrow \bar{\nu}_\mu$ neutrino oscillations in the NuMI beam at Fermilab. The NOνA experiment will mainly study the ν_e appearance signal in a ν_μ beam. The NuMI beam does not contain ν_τ; thus, the source of ν_τ in the far detector is the oscillated neutrinos mainly from $\nu_\mu \rightarrow \nu_\tau$ ($\bar{\nu}_\mu \rightarrow \bar{\nu}_\tau$). These ν_τs will produce tau leptons by charged-current interactions in the far detector, and these tau leptons will decay into muons and electrons, mimicking the signal of the NOνA far detector. In this study, we are evaluating the possible background

from the tau neutrinos for a given POT (proton on target) exposure of the detector. For this analysis, GENIE simulated far detector tau neutrino common analysis files (CAFs) used as input, and the goal is to estimate the number of tau neutrino events that survive the ν_μ far detector standard selection criteria. The expected tau neutrino background obtained from this analysis is $\sim$0.04 event/1020 POT considering maximum oscillation probability.

Reference
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A-56

Probing DNA Bending Kinetics by yNhp6A with Ultrafast Temperature Jump Spectroscopy

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The yeast Nhp6A protein is a member of the eukaryotic HMGB family of chromatin factors that enhance apparent DNA flexibility in many cellular processes. yNhp6A exhibits no sequence-specificity but binds to DNA with 1- to 10-nM affinity, sharply bending the DNA by >60° at the binding site. Previous studies on the kinetic mechanism of DNA deformation mostly remain unclear and are limited by (millisecond) time resolution. It is not known whether the protein first binds weakly to unbent DNA and then deforms the DNA or whether partially bent DNA conformations are thermally accessible and "captured" and stabilized by the bound protein. Our kinetic data show that at low salt (<250-mM NaCl) and lower temperature (<62.5°C), there is a fraction of population in which the DNA is unbent but not yet dissociated. Our equilibrium and kinetics data provide direct evidence for the proposed pathway of "bind first" and "bend second" with an intermediate where the protein is still bound to the unbent duplex. These results represent the first observation of DNA bending/unbending dynamics in complex with a nonspecific DNA-binding protein, and represent an important step toward a more comprehensive understanding of the kinetic mechanisms of DNA binding and bending interactions.

A-57

Improving Pharmaceutical Inhaler Design using Synchrotron X-ray Diagnostics

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Metered dose inhalers have been the predominant method of drug delivery to the lungs for over 50 years. They are safe and easy to use, but have many limitations. The fraction of drug actually delivered to the alveoli is only 10 to 40%, and is highly variable between uses, making them unsuitable for low-dose drugs. The low respirable fraction is due to incorrect operation by the patient, non-ideal spreading of the spray, and non-ideal particle size. These factors ultimately depend upon the design of the inhaler itself. The nozzle is small (typically 300 μm) and operates via flash evaporation of a propellant (and co-solvent) carrying the drug in suspension or solution. To understand the physical phenomena behind the limiting factors of current designs, synchrotron x-rays from the Advanced Photon Source at Argonne National Laboratory are being used. Phase contrast imaging provides a detailed view of the flow structures inside

the nozzle. Time-resolved radiography provides a quantitative measurement of the density distribution in the spray near to the nozzle, where laser scattering diagnostics fail. Finally, time-resolved fluorescence spectroscopy provides quantitative measurements of the drug distribution, independent of other constituents. This work will lead to the design of more efficient and reliable inhalers.

A-58

New Approach for Bragg Coherent Diffractive Imaging with Polychromatic X-rays

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Bragg coherent x-ray diffraction imaging (CXDI) is a powerful technique to obtain three-dimensional images as well as internal strain distributions of various types of specimens at the nanoscale [1–4]. However this technique requires significant time to perform three-dimensional scans making it incompatible with most time-resolved studies. In this study, we propose a new approach for CXDI with the goal of obtaining three-dimensional information on short time scales using polychromatic x-rays from the third generation synchrotron source. Because polychromatic coherent x-rays produce multiple projections of coherent diffraction patterns at the same time, this approach takes advantage of rapid measurements for real time and time-resolved studies. We collected slices of coherent x-ray diffraction patterns at the same time with an area detector. The setup and preliminary results taken at the 34ID-E beamline of the Advanced Photon Source will be discussed.

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A-59

Parity-Time Symmetry Breaking in Magnetic Systems

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The vast majority of natural processes, ranging from large-scale flows in the atmosphere and the evolution of ecological systems to electric charge and energy transfer in technology, occur in out-of-equilibrium conditions. However, theoretical descriptions, especially concerning the instabilities and dynamic phase transitions, are limited to a few specific situations. What hinders progress in out-of-equilibrium phase transitions is the lack of a general principle governing nonequilibrium physics. We introduce a generalized non-Hermitian Hamiltonian approach for the description of out-of-equilibrium phase transitions in the exemplary context of dissipative nonequilibrium dynamics of an open quantum spin system. The imaginary part of the proposed Hamiltonian describes effects of damping and the applied Slonczewski spin-transfer torque (STT). In the classical limit, our approach reproduces Landau-Lifshitz-Slonczewski dynamics of a large macrospin. We reveal the STT-driven parity-time (PT) symmetry-breaking transition corresponding to a phase transition from precessional magnetization dynamics to controlled switching. Micromagnetic simulations for nanoscale ferromagnetic disks demonstrate the predicted effect. Our findings break ground for a general quantitative description of out-of-equilibrium phase transitions.

A-60

The Design of Cathode Materials for Nonaqueous Mg-Battery Applications

Feng, Zhenxing, Xiao Chen, Michael J. Bedzyk, and Paul Fenter

The development of advanced multivalent batteries that have a higher energy density than current state-of-art Li-ion battery (LIB) is predicated on the identification of new chemistries, including a compatible combination of cathode, anode and non-aqueous electrolyte. Using solid-state chemistry, sputtering and pulsed laser deposition methods, we identify and control the factors that influence electrochemical activity for Mg insertion/de-insertion in Mg-based spinels through the epitaxial stabilization of such thin films in the distinct tetragonal and cubic phases, where the latter is only thermodynamically stable at high temperature (> 950°C) or high pressure (> 15.6 GPa). This comparison demonstrates that the two phases exhibit dramatically different electrochemical activity in non-aqueous electrolytes such as $MgCl_2$-, $Mg(TFSI)_2$-, and $Mg(CB_{11}H_{12})_2$-based electrolyte. Specifically, cubic phase in Mg-full cells exhibits reversible Mg^{2+} insertion and extraction with associated changes in film structure and Mn-oxidation states, while tetragonal phase has negligible charge/discharge activity. These results demonstrate the potential for multivalent cation intercalation in a spinel material in non-aqueous/non-Grignard electrolytes, and provide a new strategy for material design for next-generation battery materials.

A-61

In Situ Characterization of $Co_{1-x}Pt_x$ Bimetallic Clusters under H_2 and CO + H_2 mixture

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CoPt alloy particles have recently attracted great interests for their excellent catalytic [1, 2] and magnetic [3] properties. In situ characterization is thus essential to probe the structure and composition of bimetallic clusters under reaction conditions in a catalytic process of interest. $Co_{1-x}Pt_x$ bimetallic clusters (x = 0, 0.25, 0.5, 0.75, 1) with atomic precision were synthesized using mass-selected low energy clusters beam deposition [4] and soft-landed onto the amorphous alumina thin film prepared by atomic layer deposition [5]. The median diameter of alloy clusters is 3 nm with a size dispersion of <10% according to transmission electron microscopy. Utilizing x-ray photoemission spectroscopy, the oxidation state of as-made clusters and the aged particles after extended exposure to air was characterized. After aging, both cobalt and platinum species in the bimetallic clusters were found to be oxidized, while the shift of their valence state exhibits a nonlinear correlation with their atomic composition. Utilizing in situ grazing incidence x-ray absorption spectroscopy [6, 7, 8, 9], the evolution of the oxidation state of the alloy particles was monitored under hydrogen reduction and $CO+H_2$ mixture. The in situ characterization reveals that a low Pt/Co ratio facilitates the formation of $Co(OH)_2$, whereas a high Pt/Co ratio stabilizes

the Co_3O_4 composition instead due to the formation of Co@Pt core-shell structure, where the platinum shell inhibits the reduction of cobalt in the core of the $Co_{1-x}Pt_x$ alloy clusters.

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A-62

Simulation of the Vortex Dynamics in a Real Pinning Landscape of YBCO Coated Conductors

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We present a critical current analysis of a real high-temperature superconducting (HTS) sample in a magnetic field by combining state-of-the-art large-scale Ginzburg-Landau simulations with reconstructive three-dimensional scanning transmission electron microscopy tomography of the pinning landscape in Dy-doped $YBa_2Cu_3O_{7-\delta}$. This methodology provides a unique look at the vortex dynamics in the presence of a complex pinning landscape, responsible for the high current-carrying capacity characteristic of commercial HTS wires. Our method demonstrates very good functional and quantitative agreement of the critical current between simulation and experiment, providing a new predictive tool for HTS wires design.

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