



Argonne National Laboratory Postdoctoral Research and Career Symposium

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October 10-11, 2013

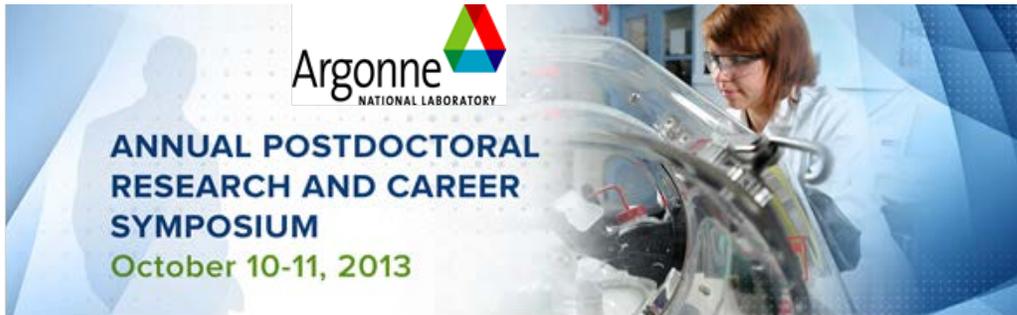


Postdoctoral Research and Career Symposium

October 10-11, 2013

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Program at a Glance

Thursday, October 10th

- 7:45 AM** **Registration—TCS Conference Center, Building 240**
- 8:30 AM** **Opening Plenary Session—Room 1416**
- Welcome Remarks:** G. Brian Stephenson, Associate Laboratory Director, Photon Sciences, Argonne Distinguished Fellow
- Introductory Remarks:** Perry Motsegood, Secretary, Postdoctoral Society of Argonne
- Keynote Address:** *Opportunities and Challenges in Research, Teaching and Leadership in Environmental Science*
 Dr. Vicki H. Grassian
 F. Wendell Miller Professor
 Department of Chemistry
 The University of Iowa
- 10:00 AM** **Concurrent Research Sessions—TCS Breakout rooms 1404, 1405, 1406**
 Oral presentations by postdoctoral and graduate student attendees
- 12:15 PM** **Working Lunch and Career Panel Discussion—Room 1416**
- Erin Dragotto**, Executive Director, Chicago Council on Science & Technology
Yash Vaishnav, Business Development Executive, Technology Development & Commercialization, Argonne National Laboratory
Jason Zielke, CTO & SVP, Clean Energy Trust
- 1:45 PM** **Career Exhibitions and Company Presentations**
- Exhibit booths in room 1416
 Presentations will begin at 2:00 PM in the TCS Breakout rooms 1404, 1405, 1406
- 4:00 PM** **Tour of User Facilities—Visualization Facility, TCS Conference Center**
- 5:15 PM** **Poster Session and Reception—APS Lower Level Gallery, Building 401**
 Flash talks will begin at approximately 5:30 PM

Special Thanks to our 2013 Sponsors!



Friday, October 11th

- 7:45 AM** **Registration/Check In—TCS Conference Center, Building 240**
- 8:30 AM** **Opening Plenary Session—Room 1416**
- Welcome Remarks:** Tina Henne, Postdoctoral Program Coordinator
- Presentation of the 2013 Outstanding Postdoctoral Mentor and Outstanding Postdoctoral Supervisor Awards**
- Winners to be announced at the Symposium
Presentation by the PSA Mentoring Committee and the Postdoctoral Program Coordinator
- 10:00 AM** **Concurrent Research Sessions—TCS Breakout rooms 1404, 1405, 1406**
Oral presentations by postdoctoral and graduate student attendees
- 12:15 PM** **Working Lunch and Career Panel Discussion—Room 1416**
- Trevis Crane**, Program Manager, Northrop Grumman (industry)
Jeff Margolis, Managing Director of the Illinois Science & Technology Coalition (science policy/federal government/nonprofit)
Joy Ramos, Account Manager/Medical Writer at Prescott Medical Communications Group (science writing)
Kapila Vigés, Director of EnterpriseWorks Chicago, University of Illinois' tech incubator in Chicago (economic development/entrepreneurship)
- 1:45 PM** **Career Exhibitions and Networking Time**
- Exhibit booths in room 1416
- 3:30 PM** **Official Program Closes**

2013 Keynote Address



Opportunities and Challenges in Research, Teaching and Leadership in Environmental Science

***Vicki H. Grassian, Ph.D.
F. Wendell Miller Professor of Chemistry
University of Iowa***

In this talk, I will discuss some of the ongoing research projects in my laboratory that focus on the surface chemistry and impacts of particles from nanometer to micrometer scales. This research involves a range of topics that include atmospheric aerosols and environmental and health impacts of nanoparticles. Drawing from my own experience as an academic chemist working across disciplines, I will also discuss the many opportunities as well as some of the challenges in research, teaching and leadership in environmental science.

Biography

Vicki H. Grassian received her B.S. degree in Chemistry from the State University of New York at Albany. From there, she did her graduate studies at Rensselaer Polytechnic Institute (M.S., 1982) and the University of California-Berkeley (Ph.D., 1987). Following postdoctoral positions, she began her independent academic career at the University of Iowa as an Assistant Professor. Professor Grassian is currently the F. Wendell Miller Professor of Chemistry in the Department of Chemistry and holds appointments in the Departments of Chemical and Biochemical Engineering and Occupational and Environmental Health. In 2006, she was appointed Founding Director of the Nanoscience and Nanotechnology Institute at the University of Iowa by the Vice President for Research. She also currently directs the Nanotoxicology Core of the NIEHS-funded Environmental Health Sciences Research Center in the College of Public Health

Professor Grassian's research interests are in the areas of environmental molecular surface science, heterogeneous atmospheric chemistry, climate impact of atmospheric aerosols, and environmental and health aspects of nanoscience and nanotechnology. She has been a pioneer in laboratory studies of the reactivity and physicochemical properties of mineral dust aerosol. These studies provide the fundamental basis needed to better understand the global impacts of mineral dust in the atmosphere. Her research has shown the importance and multiple roles that adsorbed water can play on the structure and chemistry of oxide and carbonate surfaces, two important components of mineral dust aerosol, with trace atmospheric gases. Her research on environmental applications and implications of metal and metal oxide nanoparticles as well as nanocrystalline zeolites utilizes molecular-based tools to provide insights into the surface reactivity of these materials. She spearheaded and published with collaborators the first papers on the inhalation toxicity of metal and metal oxide nanoparticles that contained full characterization data of the nanomaterials. Nanomaterial characterization is now considered an important component and requisite in these toxicity studies. She has given over 200 invited talks and presentations on her research including the 2012 Hascoe Distinguished Lecture at the University of Connecticut, and a was a keynote speaker for the 2012 Dorothy Crowfoot-Hodgkin Symposium at the University of Zurich. She has published over 240 peer-reviewed publications and 16 book chapters. She has edited three books.

At the University of Iowa, Professor Grassian has mentored over one hundred students in her laboratory including twenty-one students who have received their PhDs under her guidance. Two of her Ph.D. students received distinguished dissertation awards from the Graduate College. She has mentored and worked with nearly thirty postdoctoral and visiting scientists. Many of her students have gone on to develop research programs in energy and the environment at academic institutions and national laboratories. She has developed a number of curriculum initiatives including the chemical sciences track of the B.S. degree program in environmental science and has advised others on developing similar programs at their institutions. Because of these initiatives and her excellence in mentoring and scholarship, she has been the recipient of a number of awards and honors at the University of Iowa. These include a Faculty Scholar Award (1999-2001) a Distinguished Achievement Award (2002), a James Van Allen Natural Sciences Faculty Fellowship (2004), the Regents Award for Faculty Excellence (2006), and Outstanding Graduate Student Mentor Award (2008).

In 2003, Professor Grassian received an US-National Science Foundation Creativity Award and in 2005, she was elected as a Fellow of the American Association for the Advancement of Science. More recently, she was named a Fellow of both the Royal Society of Chemistry and the American Vacuum Society in 2010 and, in 2011, became a Fellow of the American Chemical Society. In 2012, she received the National ACS Award for Creative Advances in Environmental Science and Technology for her original and creative contributions in understanding mineral dust aerosol properties through laboratory studies and their impact on atmospheric chemistry and climate.

Dr. Grassian currently lives in Iowa City, Iowa with her husband, Mark Young, and two daughters, Alexandra and Samantha. She enjoys spending her free time with her family and taking walks with her dog Sniggles.

Welcome Remarks



G. Brian Stephenson, PhD

Associate Laboratory Director, Photon Sciences and the Director of the Advanced Photon Source (APS), Argonne National Laboratory

Dr. Stephenson's research interests focus on developing and using synchrotron X-ray techniques to understand materials synthesis and processing. He has extensive experience in building and managing synchrotron X-ray instrumentation and beamlines, and was the recipient of an R&D 100 Award for his work on the Hard X-Ray Nanoprobe beamline at APS. Prior to becoming director in 2010, he had been involved for many years in carrying out research at APS and in developing the proposal to upgrade the APS.

Dr. Stephenson joined the staff of Argonne's Materials Science Division in 1995. Previously he was a research staff member and group leader at IBM Research in Yorktown Heights, NY. He is co-author of more than 150 publications, and a Fellow of the American Physical Society. He received B.S. and M.S. degrees in 1978 from the Massachusetts Institute of Technology, and a Ph.D. in 1983 from Stanford University.



Perry N Motsegood, PhD

Secretary, Postdoctoral Society of Argonne

Perry Motsegood is a Postdoctoral Appointee in the Chemical Sciences and Engineering Division at Argonne National Laboratory. He is the current Secretary for the Postdoctoral Society of Argonne. He received his doctorate in chemistry from the University of Iowa in electrochemistry, where he investigated magnetic enhancement of electrochemical systems and developed breath sensors for the detection acetone. He is currently a member of the Nuclear and Environmental Processes Department where he applies his electroanalytical skills toward the development of pyrochemical processes for used nuclear fuel. As the Secretary of the Postdoctoral Society of Argonne, Perry helps steer PSA organizational activities, including the annual Research and Career Symposium.



Laura Zamboni, PhD

Chairperson, Postdoctoral Society of Argonne Mentoring Committee

Laura Zamboni is a Climate Scientist and Computational Postdoctoral Fellow in the Mathematics and Computer Sciences Division. She received her "Laurea" Masters of Science in Physics from the Università degli Studi di Bologna and her Ph.D. in Environmental Fluid Mechanics from Università degli Studi di Trieste. Currently she is using Intrepid at the Argonne Leadership Computing Facility to investigate the sensitivity and uncertainty of precipitation in climate models. Using high-resolution models, her research is furthering the risk assessments and water management worldwide. Laura is also expanding scientific knowledge and understanding of processes in cloud formation and precipitation.

Career Panel Speakers



Erin Dragotto, BS, MA
Executive Director, Chicago Council on Science and Technology (C²ST)
Founder, President, Chicago Teen Museum

Erin Dragotto is originally from Manhattan, Kansas, and studied Liberal Arts at Pepperdine University, Malibu, CA. In 2003 she began her Master's degree in art education from the School of the Art Institute of Chicago. During this time, she accepted a position with the Adler Planetarium & Astronomy Museum where she worked as a museum educator and lead on the NASA funded *Global Climate Change* forum series, which helped to bring the Chicago Council on Science and Technology to fruition. Erin serves as Founder and President of The Chicago Teen Museum (CTM), a non-profit organization dedicated to bridging teen creativity with the museum profession; is a member of the Young Professionals for Non-Profits and Chicago Council on Global Affairs; and represents the Chicago Council on Science and Technology on the former Mayor Daley's - Mayors Council of Technology Advisors. As an art educator with a focus on the educational impacts of non-profit art institutions, Erin brings her knowledge of museums and non-profit management in her current position to create a dynamic organization that will affect the greater scientific community in Chicago. Erin holds a bachelor's degree from Pepperdine University in Malibu, a Masters of Art in Art Education from the School of the Art Institute of Chicago, and completed a Project Management certification from the University of Chicago, Graham School.



Yash Vaishnav, PhD, MBA
Business Development Executive, Technology Development & Commercialization
Argonne National Laboratory

Yash Vaishnav manages technologies in a variety of areas including life sciences, nanotechnology, bioprocessing, catalysis and energy sciences. He also leads business development activities to build long-term and strategic relationship with industry. Yash mentors Argonne-based startup companies and supports various laboratory research funding programs. He has 25 years of experience in scientific research, intellectual property management, technology transfer, and business development. Prior to joining Argonne in 2008, he worked at the UC San Diego School of Medicine, the International Center for Genetic Engineering & Biotechnology (ICGEB), New Delhi, Knobbe, Martens, Olson, and Bear, LLP (an IP law firm), the system-wide Office of Technology Transfer in the UC Office of President, and the Office of Intellectual Property & Industry Sponsored Research at UCLA. He has extensive experience in technology assessment, patenting, marketing, licensing, and industry partnership. Yash has a Ph.D. in Molecular Biology from the Indian Institute of Science, Bangalore, and an MBA in finance from California State University. He is active in the local venture capital community, Chicago Innovation Mentors, and supports a business plan competition at Booth School of Business at the University of Chicago.



Jason Zielke, MBA
Senior VP and CTO, Clean Energy Trust (CET)

Jason Zielke has developed strategy, operations, programs and personnel to grow the organization from a concept into a company that now has 8 full time employees. Under his leadership CET has developed a set of offerings and services which have helped to facilitate over \$38M in follow on funding to clean energy entrepreneurs. Jason is the principal point of contact within the organization for CET's commercialization activities, including managing CET's role with the DoE Energy Storage Hub, a \$120M public-private partnership. And the consulting practice that he has built with CET includes clients in the military, oil and gas, energy storage, real estate development and specialty chemicals businesses. Prior to the Clean Energy Trust, Jason was a Venture Associate at Dillon Kane Group, a Chicago based advisory firm, where he evaluated potential cleantech and software investments, and supported the development of 4 new companies, including an aviation software company and a battery technology company that he co-founded. He began his career as a chemical engineer at UOP. He has a B.S in Chemistry from Southern Illinois University, an M.S. in Chemical Engineering from the University of Tennessee, where he was also research associate at Oak Ridge National Laboratory. He earned his MBA from The University of Chicago Booth School of Business.



Trevis Crane, PhD
Program Manager, Northrup Grumman

In 2005 Trevis Crane received his Ph.D. in physics from UIUC studying $1/f$ noise at low temperatures in superconductors. Subsequently, he completed a postdoctoral research position, also at UIUC. In 2007, Dr. Crane moved to the northwest suburbs of Chicago to begin work at Northrup Grumman Corporation as a systems engineer. After two years of rotating through the various sub-disciplines of systems engineering (requirements analysis, algorithm development, and integration and test), he moved into project management, eventually finding a home in late 2010 as a program manager for Infrared Countermeasure (IRCM) development programs, managing both internally funded and customer funded R&D efforts.



Jeffrey Margolis, PhD
Managing Director, Illinois Science and Technology Coalition

Jeffrey Margolis brings twelve years of experience across the technology commercialization pipeline to the role of Managing Director at the Illinois Science and Technology Coalition. As Managing Director, he focuses on strategic planning and partnership building to support key ISTC initiatives that leverage research and development activities to promote economic development in the State of Illinois. Prior to joining the ISTC, Jeff worked in the Office of Science & Technology Cooperation at the U.S. Department of State developing technology innovation and entrepreneurship programs in emerging markets. As a life scientist, he performed translational research at Baxter International, Pfizer, and Lawrence Livermore National Laboratory. Jeff also served as a founding Vice President of Development for

CollegeSpring, an education nonprofit that serves low-income communities throughout California. Jeff holds a PhD from Stanford University, a BA from Northwestern University, and is a graduate of the Illinois Mathematics and Science Academy.



Joy Ramos, PhD
Account Manager & Medical Writer, Prescott Medical Communications Group

Joy received her Ph.D. in Cell Biology from Northwestern University and her B.S. in Molecular Biology and Biotechnology from the University of the Philippines. She enjoys sharing her enthusiasm about science with the general public and has been involved with various science outreach opportunities in the Chicagoland area. She has been an active member of the Association for Women in Science - Chicago chapter (AWIS Chicago) for many years and currently serves as its Immediate Past President, in addition to being a longtime contributor to the national AWIS magazine.



Kapila Vigés, Materials Science and Engineering
Director, EnterpriseWorks Chicago, University of Illinois

As the Director of EnterpriseWorks Chicago, Kapila Vigés builds on the successes of EnterpriseWorks, the tech incubator on the Urbana campus. EnterpriseWorks supports startup companies with an array of programs, facilities, activities, and events designed to nurture entrepreneurship and company formation. She was previously Director of Entrepreneurship and Innovation at the Michigan Economic Development Corporation, where she led statewide entrepreneurial programs of the Michigan 21st Century Jobs Fund. Vigés received her degree in Materials Science and Engineering from Johns Hopkins University.

Outstanding Postdoctoral Mentor and Outstanding Postdoctoral Supervisor Award Recipients

The Postdoctoral Society of Argonne (PSA), together with the Postdoctoral Program Office and the Office of the Director is pleased to announce the recipients of the Inaugural Outstanding Postdoctoral Mentor and Outstanding Postdoctoral Supervisor Awards. Spearheaded by the PSA Mentoring Committee, these awards recognize the efforts of Argonne staff who serve as strong advocates for Postdocs inside and outside the lab, provide consistent professional guidance, contribute to an environment that boosts curiosity, passion and performance and enrich the postdoctoral experience.



Jimmy Proudfoot (HEP)

Cristina Negri (ES)

Jimmy Proudfoot (HEP) is the recipient of the 2013 Outstanding Postdoctoral Mentor Award. Cristina Negri (ES) is also recognized with an Honorable Mention in this category. Both individuals are recognized for demonstrating strong advocacy for professional skills development, collaboration inside and outside the laboratory and providing guidance through career path decisions.



Daniel Abraham (CSE)

Igor Aronson (MSD)

Daniel Abraham (CSE) and Igor Aronson (MSD) will share the 2013 Outstanding Postdoctoral Supervisor Award. Both supervisors demonstrated outstanding qualities in mentoring and supervision of postdocs, including discussing career options, advocating inside and outside the laboratory and promoting postdoc achievements to enhance postdocs' reputations within their disciplines and to a broader audience. These award recipients are also exemplars of strengthening the science, technology, engineering and mathematics (STEM) pipeline.

Special Thanks to the Outstanding Postdoctoral Mentor and Supervisor Award Committee for their hard work on this important initiative.

Laura Zamboni (MCS), Computational Fellow, PSA Board Member and Mentoring Committee Chairperson

Diego Fazi (CSE), Postdoctoral Appointee, PSA Board Member and Mentoring Committee Member

Joseph Bernstein (HEP), Past PSA Liaison Officer, Mentoring Committee Member

Katie Carrado-Gregar, Manager of CNM User & Outreach Programs, 2006 DOE Outstanding Mentor Award Recipient

John Schlueter (MSD), Chemist, 2004 DOE Outstanding Mentor Award Recipient

Erin Thomas (OTD), Gender Diversity Specialist

Tina Henne (CEPA), Postdoctoral Program Coordinator



**Argonne National Laboratory
Postdoctoral Research Symposium**

SUMMARY OF SESSIONS

October 10, 2013

Session	Session Title/Chairpersons	Start Time	End Time	Location
1	Engineering Design and Applications Christopher Annesley	10:00 AM	12:00 PM	1404
2	Materials Synthesis and Development Shalaka Desai	10:00 AM	12:00 PM	1405
3	Physics and High Energy Physics Cong Liu	10:00 AM	12:00 PM	1406

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4	Simulation, Algorithms and Modeling Samrat Saha	10:00 AM	12:00 PM	1404
5	Structure Characterization Ujjal Das	10:00 AM	12:00 PM	1405
6	Chemistry and Biosciences Laura Zamboni	10:00 AM	12:00 PM	1406

ORAL PRESENTATIONS

Building 240

Thursday, October 10, 2013

Session 1: Engineering Design and Applications **Room 1404**
Session Chair: Christopher Annesley

- 10:00 AM DEVELOPMENT OF A PROTOTYPE CALIBRATION SYSTEM FOR THE LBNE PHOTON DETECTION SYSTEM
Sahoo, Himansu, Djurcic, Zelimir, Drake, Gary, High Energy Physics Division, Argonne National Laboratory, Argonne, IL 60439
- 10:20 AM GOLD-ZNO NANO-COMPOSITES AS CATALYTIC ADSORBENTS FOR LOW-TEMPERATURE REACTIVE DESULFURIZATION
Behl, Mayank¹, Jain, Prashant², ¹Chemical and Biomolecular Engineering Department, University of Illinois at Urbana-Champaign, Urbana, IL 61801; ²Chemistry Department, University of Illinois at Urbana-Champaign, Urbana, IL 61801
- 10:40 AM RUBIDIUM-PROMOTED MOLYBDENUM CARBIDE CATALYSTS FOR MIXED ALCOHOL SYNTHESIS FROM SYNGAS
Shou, Heng¹; Davis, Robert J. ²; ¹Chemical Sciences and Engineering Division, Argonne National Laboratory, Argonne, IL 60439; ²Department of Chemical Engineering, University of Virginia, Charlottesville, VA 22904
- 11:00 AM GUIDING THE FORMATION OF SINGLE-HANDED ENANTIOMERIC PORPHYRIN DOMAINS USING KINKED AND CHIRAL STEPPED SURFACES
Avila-Bront, L. Gaby; Fleming, Christopher, D.; Whitfield, Mark C.; Kautz, Natalie, A. Sibener, Steven J. Chemistry Department, The University of Chicago, Chicago, IL 60637
- 11:20 AM VISUALIZATION OF INDIVIDUAL DEFECT MOBILITY AND ANNIHILATION WITHIN CYLINDRICAL DIBLOCK COPOLYMER THIN FILMS ON NANOPATTERNED SUBSTRATES
Tong, Qianqian; Sibener, Steven J., Chemistry Department, The University of Chicago, Chicago, IL 60637
- 11:40 AM DEVELOPMENT OF NANOSILICON-POLYANILINE CAPSULES FOR RENEWABLE ENERGY APPLICATION
Maximenko, Yulia¹; Elhalawany, Noha²; Yamani, Zain³; Yau, Siu-Tung⁴; Nayfeh, Munir¹, ¹Physics Department, University of Illinois at Urbana-Champaign, Urbana, IL 61801, ²National Research Center, Cairo, Egypt, ³Center of Excellence for Nanotechnology, KFUPM, Chahran, Saudi Arabia, ⁴Cleveland State University, Cleveland, OH 44115
- 12:00 PM Lunch and Career Panel Discuss – Room 1416

Session 2 Materials Synthesis and Development Room 1405

Session Chair: *Shalaka Desai*

- 10:00 AM TUNING TUNGSTEN-ALKYLIDYNE/ZINC-PORPHYRIN DONOR-ACCEPTOR DYADS TO POWER CO₂ REDUCTION
O'Hanlon, Daniel; The University of Chicago, Chicago, IL 60637
- 10:20 AM STABILIZING CU₂S PHOTOVOLTAICS VIA ULTRATHIN ALD BARRIER LAYERS
Riha, Shannon C.; Martinson, Alex B. F., Materials Science Division, Argonne National Laboratory, Argonne, IL 60439
- 10:40 AM PROLONGING LIFE OF HIGH ENERGY LITHIUM-ION CELLS
Bettge, Martin; Li, Yan; Zhu, Ye; Abraham, Daniel P., Chemical Sciences and Engineering Division, Argonne National Laboratory, Argonne, IL 60439
- 11:00 AM DESIGNING SOLUBLE PRECURSORS FOR THIN-FILM PHOTOVOLTAICS
Jiang, Chengyang; Talapin, Dmitri V., Chemistry Department, The University of Chicago, Chicago, IL 60637
- 11:20 AM TA_{0.3}TI_{0.7}O₂ ELECTROCATALYST SUPPORTS EXHIBIT EXCEPTIONAL ELECTROCHEMICAL STABILITY
Kumar, Amod; Ramani, Vijay, Department of Chemical and Biological Engineering, Illinois Institute of Technology, Chicago, IL 60616
- 11:40 AM MESOSCALE MODELING OF ELECTROCHEMICAL CRYSTAL GROWTH FOR ADVANCED LITHIUM BATTERIES
Welland, Michael J.; Wolf, Dieter, Materials Science Division, Argonne National Laboratory, Argonne, IL 60439
- 12:00 PM Lunch and Career Panel Discuss – Room 1416

Session 3: Physics and High Energy Physics

Room 1406

Session Chair: *Cong Liu*

- 10:00 AM HIGH PRESSURE GAS-FILLED CAVITIES FOR USE IN A MUON COOLING CHANNEL
Freemire, Ben T.¹, Tollestrup, Alvin V.²; Yonehara, Katsuya²; Chung, Moses²; Torun, Yagmur¹, ¹Physics Department, Illinois Institute of Technology, Chicago, IL 60616; ²Fermi National Accelerator Laboratory, Batavia, IL 60610
- 10:20 AM INVESTIGATING THE ROLE OF MAGNETIC INTERACTIONS IN METAL-INSULATOR TRANSITION OF LAYERED IRIDATE SR₂IR₄O₄
Chikara, Shaline¹; Fabbris, Gilberto²; Qi Tongfei³, Terzic, Jasminka³, Cao, Gang³, Haskel, Daniel³, ¹X-Ray Science Division, Argonne National Laboratory, Argonne, IL 60439, ²Physics Department, Washington University, St. Louis, MO 63130, ³Center for Advanced Materials and Physics Department, University of Kentucky, Lexington, KY 40506
- 10:40 AM STUDYING EXOTIC NUCLEI USING A NEW FAST BETA-DECAY TAGGING SYSTEM AT ARGONNE
David, Helena M., Physics Division, Argonne National Laboratory, Argonne, IL 60439
- 11:00 AM SUPERCONDUCTING VORTEX PINNING VIA NANOPATTERNING
Wang, Y.L.¹, Xiao, Z.L.¹, Divan, R.², Ocola, L.E.², Crabtree, G.W.¹, Kwok, W.K.¹
¹Materials Science Division, Argonne National Laboratory, Argonne, IL 60439;
²Nanoscience and Technology Division, Argonne National Laboratory, Argonne, IL 60439

- 11:20 AM ORBITAL ANGULAR MOMENTUM OF PHOTONS AND HIGH-HARMONIC GENERATION
Picón, Antonio, X-Ray Science Division, Argonne National Laboratory, Argonne, IL 60439
- 11:40 AM COEXISTENCE OF TWO DIFFUSION MECHANISMS: W ON W(100)
Olewicz, Tomasz¹; Ehrlich, Gert²; Lyding, Joseph W.¹; Antczak, Grażyna³
¹Department of Electrical and Computer Engineering, University of Illinois at Urbana-Champaign, Urbana, IL 61801; ²Materials Research Laboratory, University of Illinois at Urbana-Champaign, Urbana, IL 61801, ³Institute of Experimental Physics, University of Wrocław, Wrocław Poland
- 12:00 PM Lunch and Career Panel Discuss – Room 1416

Friday, October 11, 2013

Session 4 **Simulation, Algorithms and Modeling (SAM)** **Room 1404**
Session Chair: **Samrat Saha**

- 10:00 AM A LEARNING ALGORITHM FOR SPACE MAPPING AND SEARCHING USING ADAPTIVE MESH REFINEMENT
Phillips, Carolyn L., Mathematics and Computer Science Division, Argonne National Laboratory, Argonne, IL 60439
- 10:20 AM MODELING CENTRAL CARBON CORE METABOLISM IN MICROBIAL LIFE
Edirisinghe, Janaka N.; Conrad, Neal, Xia, Fangfang; Overbeek, Ross; Henry, Christopher S., Mathematics and Computer Science Division, Argonne National Laboratory, Argonne, IL 60439
- 10:40 AM TOWARDS OPTIMAL WORKFLOW TO SUPPORT MASSIVELY PARALLEL IMPLICIT ADAPTIVE COMPUTATIONAL FLUID DYNAMICS SIMULATIONS ON COMPLEX GEOMETRIES
¹Rasquin, Michel; ²Smith, Cameron; ³Chitale, Kedar; ²Seol, Seegyoung; ³Matthews, Benjamin; Sahni, Onkar; Shephard, Mark; Jansen, Kenneth; ¹Leadership Computing Facility, Argonne National Laboratory, Argonne, IL 60439; ²Rensselaer Polytechnic Institute, Troy, NY 12180; ³University of Colorado-Boulder, Boulder, CO 80309
- 11:00 AM LEADER SELECTION IN CONSENSUS NETWORKS
¹Lin, Fu; ²Fardad, Makan; ³Jovanovic, Mihailo M., ¹Mathematics and Computer Science Division, Argonne National Laboratory, Argonne, IL 60439; ²Syracuse University, Syracuse, NY 13244; ³University of Minnesota, Minneapolis, MN 55455
- 11:20 AM URANYL(VI) AND PLUTONYL(VI) COORDINATION AND DYNAMICS IN A TASK-SPECIFIC IONIC LIQUID
Maerzke, Katie A.; Schneider, William F.; Maginn, Edward J.; Chemical and Biomolecular Engineering Department, University of Notre Dame, Notre Dame, IN 46556.
- 11:40 AM TRANSPORTED PDF MODELLING OF SPRAY COMBUSTION AT DIESEL ENGINE CONDITIONS
Yuanjiang Pei¹; Evatt R. Hawkes²; Sanghoon Kook²; Sibendu Som¹; ¹Energy Systems Division, Argonne National Laboratory, Argonne, IL 60439, ²University of New South Wales, Sydney, Australia
- 12:00 PM Lunch and Career Panel Discuss – Room 1416

Session 5 **Structure Characterization**
Session Chair: **Ujjal Das**

Room 1405

- 10:00 AM KIRKPATRICK-BAEZ MIRRORS TO FOCUS HARD X-RAYS IN 2-D ARE FABRICATED, TESTED, AND INSTALLED AT THE ADVANCED PHOTON SOURCE
Naresh Kujala; Shashidhara Marathe; Deming Shu; Bing Shi; Jun Qian; Lydia Finney; Chris Jacobsen; Albert Macrander; Lahsen Assoufid; X-Ray Science Division, Argonne National Laboratory, Argonne, IL 60439
- 10:20 AM ATOMIC LAYER DEPOSITION OF METAL SULFIDES FOR HIGH PERFORMANCE LITHIUM BATTERIES
Meng, Xiangbo, Elam, Jeffrey, Energy Systems Division, Argonne National Laboratory, Argonne, IL 60439
- 10:40 AM SYNCHROTRON X-RAY STUDIES OF THIN FILM SOLID OXIDE FUEL CELL CATHODES
Hopper, E. Mitchell; Ingram, Brian J.; Chang, Kee-Chul; Baldo, Peter M.; You, Hoydoo; Eastman, Jeffrey A., Fuoss, Paul. H.; Materials Science Division, Argonne National Laboratory, Argonne, IL 60439
- 11:00 AM ATOMIC LAYER DEPOSITION OF IN_2S_3 VIA A NOVEL INDIUM AMIDINATE PRECURSOR
McCarthy, Robert F. ¹; Weimer, Matthew²; Pellin, Michael J. ¹; Hock, Adam S. ²; Martinson, Alex B. F. ¹; ¹Materials Science Division, Argonne National Laboratory, Argonne, IL 60439, ²Chemistry Department, Illinois Institute of Technology, Chicago, IL 60616
- 11:20 AM PROBING CHEMICAL REACTIVITY AND STRUCTURAL DEFECTS IN NIOBIUM CAVITIES: IMPROVING THE NEXT GENERATION OF PARTICLE ACCELERATORS
Kautz, Natalie A.; Gibson, Kevin D.; Nakayama, Miki; Wang, Tuo; Sibener, Steven, J.
- 11:40 AM AUTOMATED ^{18}F LABELING OF SUCROSE FOR TRANSPORTER STUDIES IN PLANTS VIA AUTORADIOGRAPHY AND PET
¹Rotsch, David; ²Brossard, Thomas; ²Ying, Waylon; ²Gaddam, Vikram; ³Swyers, Nathan; ²Harmata, Micheal; ²Cutler, Cathy; ²Robertson, David; ²Jurisson, Silvia S.; ²Braun, David; ¹Chemical Sciences and Technology Division, Argonne National Laboratory, Argonne, IL 60439, ²Chemistry Department, University of Missouri, Columbia, MO 65211, Biology Department, University of Missouri, Columbia, MO 65211
- 12:00 PM Lunch and Career Panel Discuss – Room 1416

Session 6: **Chemistry and Biosciences**
Session Chair: **Laura Zamboni**

Room 1406

- 10:00 AM HAFNIUM CLUSTER CHEMISTRY: TOWARD SCALABLE MATERIALS DESIGN, DISCOVERY, AND CREATION
Kalaji, Ali, Soderholm, Lynda, Chemical Sciences and Technology Division, Argonne National Laboratory, Argonne, IL 60439
- 10:20 AM THE IMPACT OF PSEUDOMONAS FLUORESCENS STRAINS ON ASPEN GROWTH DURING PHOSPHORUS AND NITROGEN LIMITATION
Shalaka Desai, Peter Larsen, Frank Collart; Biosciences Division, Argonne National Laboratory, Argonne, IL 60439

- 10:40 AM A SHOCK TUBE LASER SCHLIEREN STUDY OF NITROMETHANE DISSOCIATION: LOOKING FOR NEW PATHWAYS
Annesley, Christopher J.; Tranter, Robert S.; Chemical Sciences and Technology Division, Argonne National Laboratory, Argonne, IL 60439
- 11:00 AM ENHANCING CHEMICAL REACTIONS IN A CONFINED HYDROPHOBIC ENVIRONMENT: A NMR STUDY OF BENZENE HYDROXYLATION IN CARBON NANOTUBES
¹Zhang, Hongbo, Pan, ²Xiulian, ²Bao, Xinhe; ¹Chemical Sciences and Technology Division, Argonne National Laboratory, Argonne, IL 60439, Dalian Institute of Chemical Physics, Dalian China
- 11:20 AM PAIR DISTRIBUTION FUNCTION TECHNIQUES FOR THE STRUCTURAL CHARACTERIZATION OF SOLAR FUELS CATALYSTS AND A NEW ALGORITHM FOR AUTOMATIC MODEL FITTING: PDFIT
Fazi, Diego; Tiede, David, M.; Chemical Sciences and Engineering Division, Argonne National Laboratory, Argonne, IL 60439
- 11:40 AM DYNAMIC OF RU-CL SOLVENT EXCHANGE AND ITS ROLE IN CATALYTIC WATER OXIDATION BY [RU(BPY)(TRY)CL]⁺ CATALYST
Dooshaye Moonshiram, Vatsal Purohit, Igor Alperovich, Ruifa Zong, Randolph P. Thummel, Yulia Pushkar; Department of Physics, Purdue University-West Lafayette, IN 47906
- 12:00 PM Lunch and Career Panel Discuss – Room 1416



**Argonne National Laboratory
Postdoctoral Research and Career Symposium**

ABSTRACTS

ORAL PRESENTATIONS



A SHOCK TUBE LASER SCHLIEREN STUDY OF NITROMETHANE DISSOCIATION: LOOKING FOR NEW PATHWAYS

Nitromethane is used as a fuel or fuel additive in many different engines for specialized applications. Nitromethane also serves as the precursor for many experiments used to determine the fundamental kinetics of NO_x chemistry. The complex system of reactions and rates are used in comprehensive models for combustion such as GRI-Mech.1 Understanding the experiments from where the rates were derived requires knowledge of the rates of dissociation, and products formed. Previous experiments have studied the pyrolysis relatively thoroughly, assuming a single reaction, rxn (1). Theoretical searches have found other pathways through first order transition states (reaction 2) all of which have transition states whose energies are too high to compete.

- (1) $\text{CH}_3\text{NO}_2 \rightarrow \text{CH}_3 + \text{NO}_2$
- (2) $\text{CH}_3\text{NO}_2 \rightarrow \text{CH}_3\text{ONO}$
- (3) $\text{CH}_3\text{ONO} \rightarrow \text{CH}_3\text{O} + \text{NO}$
- (4) $\text{CH}_3\text{ONO} \rightarrow \text{CH}_2\text{O} + \text{HNO}$

Recent theoretical work by Zhu et al. has found lower energy pathways associated with reactions (2) and (4)² which belong to a new class of reactions referred to as roaming reactions. The roaming isomerization pathway to methyl nitrite (rxn 2) may compete with reaction (1) as it is lower in energy, as opposed to the first order transition state which is almost 10 kcal/mol higher in energy. Further, the methyl nitrite is assumed to dissociate through reaction (3) forming a methoxy radical and NO. However, Zhu et al. also found the possibility of a second roaming pathway to molecular dissociation, reaction (4),² which has not been seen before experimentally. The possibility of secondary products is an important problem to explore, as no other experimental study has considered these pathways. A unique ability to study this reaction is available with the diaphragmless shock tube laser schlieren technique, which will be discussed. This technique provides temperature and pressure dependent rate constants and can show branching between the various channels. Nitromethane is especially well suited to this technique as the various channels are expected to be strongly pressure dependent. Data has been taken at many different concentrations and temperature ranges allowing for models of the rate of reaction (1) to be constructed that will work at all pressures. There is also vibrational relaxation information that results from induction delays in the data which is pressure, temperature, and concentration dependent. Further, contained in this data is the branching fraction to the other possible products, which will be discussed.

Authors: Annesley, Christopher, J.; Tranter, Robert, S
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GUIDING THE FORMATION OF SINGLE-HANDED ENANTIOMERIC PORPHYRIN DOMAINS USING KINKED AND CHIRAL STEPPED SURFACES

Surface chirality can exist as either externally imposed or intrinsic to the surface facets. Molecules that are achiral in the gas phase can form organizationally chiral arrays. The chirality of such an array exists as a racemic (equal portions of left- and right-handed domains) mixture on a flat surface without the presence of many defects.¹ On the other hand, intrinsically chiral surfaces derive their chirality from the presence of defects along their step edges. These kinks expose microfacets of three surface planes. The kink sites are designated a handedness based on the rotational progression of the microfacets.² Chiral surfaces have proven to be a realistic method for not only the separation of enantiomers. Studies have shown that chiral surfaces participate in enantiospecific chemistry when molecules of matching handedness are adsorbed.³ Metalloporphyrin arrays have been previously imaged in ultrahigh vacuum (UHV) conditions with scanning tunneling microscopy (STM). The versatility of such arrays is due to their stability over a large temperature range and the possibility to functionalize their end groups and create a wide variety of two dimensional arrays. In our experiments, the self-assembly of nickel tetraphenyl porphyrin (NiTPP) on achiral Au(111), which includes randomly located kinked steps, and chiral Au(1036 1070 1035) and (1036 1035 1070) surfaces has been studied using ultrahigh vacuum scanning tunneling microscopy (UHV-STM).

Authors: Avila-Bront, L. Gaby; Fleming, Christopher, D.; Whitfield, Mark, C.; Kautz, Natalie, A.; Sibener, Steven, J.
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GOLD-ZNO NANO-COMPOSITES AS CATALYTIC ADSORBENTS FOR LOW-TEMPERATURE REACTIVE DESULFURIZATION

Sulfur compounds occur as a natural contaminant in all the major fuel feedstock including crude oil, coal, natural gas and biomass-derived syngas. These impurities are often associated with problems like equipment corrosion, downstream catalyst poisoning, and environmental pollution. Accordingly, the sulfur content in the fuel is often strictly regulated by environment-protection agencies around the world. One way of removing sulfur is to use solid adsorbents to selectively separate sulfur-components from raw fuel. Metal oxides are typically used for reactive adsorption of such organo-sulfur compounds. Poor reaction kinetics, however, requires high operating temperatures (>400°C), which results in large energy costs accompanied with chemical reduction and physical degradation of the adsorbent, resulting in lower capacity and underutilization of the adsorbent¹⁻³. As a consequence, developing adsorbents that can have high-sulfur removal capacity at low-temperature is

highly desirable. Zinc oxide is known for its favorable thermodynamics for its reaction with sulfur containing compounds, which provides it with high sulfur-removal capacity. However, sluggish kinetics of this fluid-solid reaction ($\text{ZnO} + \text{C}_x\text{H}_z\text{S}_y \rightarrow \text{ZnS}$) does not favor low temperature application, which necessitates use of a catalyst for accelerating reaction. With the objective of developing such low-temperature sorbents, I am currently investigating the potential role of noble metals as catalysts that can synergistically enhance the reactivity of a host metal oxide towards organo-sulfur impurities. Nanometer-sized gold has recently proven to be an efficient heterogeneous catalyst with high catalytic activity for selective reduction/oxidation reactions including CO oxidation, selective hydrocarbon oxidation, methanol synthesis, water-gas shift reaction and hydrogenation reactions. Gold is the only known metal to reversibly adsorb H_2S , a common sulfur impurity in the raw syngas or natural gas feedstock. Well-dispersed nano-sized gold is thought to have strong interaction with the supporting metal oxide. It has been proposed in theory, as early as 1988, that metal can change the defect equilibrium of metal oxides making them more reactive⁴. It should be noted here that in bulk of the literature, effect of this metal-metal oxide interaction has been studied only with respect to chemical reactions happening at the surface with bulk of the metal oxide remaining unreacted. In this study, the entire bulk of ZnO undergoes a solid-state transition to form ZnS. Moreover, the reaction of sulfur containing molecule with Au-ZnO has not been studied before. Thus this study hopes to not only make the catalyst composites more practical for applications involving reactive adsorption where bulk oxide undergo reactive transition (entailing higher adsorption capacity), it also aims to investigate the underlying phenomenon of oxide - metal interaction in context to its effect solid-state reactivity, an area that has not caught researcher's attention. The model system of Au-ZnO nanocomposites were chosen for above-mentioned reasons. The reaction that is being investigated involves thioacetamide as a model-sulfur containing organic molecule. The reactive performance is examined by monitoring the rate of disappearance of ZnO and extent of ZnS formed in a given time.

Authors: Behl, Mayank

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PROLONGING LIFE OF HIGH ENERGY LITHIUM-ION CELLS

For lithium-ion batteries to widely power plug-in hybrid electric and all-electric vehicles, they must meet a range of stringent criteria: for instance, energy densities high enough to allow tens of miles of travel autonomy at low initial costs; as well as consistent power densities throughout the entire state-of-charge (SOC) range. Good safety characteristics, a calendar-life of around 10 years, and a cycle-life of up to a few thousand charge and discharge cycles are also crucial. Large-scale implementation of state-of-the-art LiCoO₂-based batteries, which are widely found in small consumer electronic devices, into automotive drivetrains is limited by relatively high materials costs and low energy densities. However, advanced batteries containing lithium- and manganese-rich layered oxides (LMR-NMCs) as positive electrode materials promise to meet some of the requirements. These layered transition metal oxides show oxide-specific charge and energy densities exceeding 250 Ah-kg⁻¹ and 900 Wh-kg⁻¹ when charged beyond 4.5V vs. Li⁺/Li. Unfortunately, significant energy fade occurs when these materials are repeatedly cycled or held at such high voltages in practical, electrochemical full-cells. Because of the inherent complexity in these Li-ion cells, an all-inclusive engineering approach is essential to prolong their operational life.

In this presentation, a particularly relevant system containing Li_{1.2}Ni_{0.15}Mn_{0.55}Co_{0.1}O₂-based positive and graphitic negative electrodes is highlighted. The performance degradation for this system, i.e. its energy and power fade, is caused by capacity loss, impedance rise, and voltage fade. Using a range of complementary electrochemical and also physicochemical techniques, it was found that capacity fade is caused primarily by Li-trapping on the negative electrode, while cell impedance rise comes predominantly from the positive electrode. The contribution of voltage fade, which is triggered by irreversible structural changes within the layered oxide, is also discussed. Having identified the major sources for performance degradation, cell life is effectively prolonged by adjustment of the voltage windows over which electrochemical cycling occurs, and by various ex-situ and in-situ modifications of the electrodes. Examples of such modifications include thin alumina coatings, electrochemically-active electrolyte additives, and altered electrode formulations. Finally, some general design principles leading to cell life extension are proposed.

Authors: Bettge, Martin; Li, Yan; Zhu, Ye; Abraham, Daniel P.

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INVESTIGATING THE ROLE OF MAGNETIC INTERACTIONS IN METAL-INSULATOR TRANSITION OF LAYERED IRIDATE Sr₂IrO₄

Transition metal oxides are usually characterized by strong electron-electron interaction and cannot be described by a single particle picture and need to be treated as a many body problem. The comparable and therefore competing energy scales in these materials result in novel emergent phenomena such as high temperature superconductivity and giant magneto resistance (GMR) and holds the promise to yet more undiscovered phases. Recently, the spin-orbit coupled Iridium-based layered oxides have generated significant interest due to the prediction and observation of new electronic states. These 5d oxides are expected to be more metallic compared to the 3d and 4d oxides because of their more spatially extended orbitals. Notably though, most iridates including Sr₂IrO₄, Sr₃Ir₂O₇ and NaIrO₃ show insulating behavior defying this conventional perception. As it turns out, the strong SOI in the heavy iridates causes band splitting resulting in narrow bands and stronger correlations. I

present the results of our X-ray spectroscopy measurements on Rh and Ru substituted Sr₂IrO₄. The metal to insulator transition in these systems was believed to be a result of decreased SOI due to replacing Ir by lighter Rh and Ru ions. We do not see any evidence to support this in our results. We see a change in the oxidation state of the dopant with increasing concentration which might be at the heart of the metallic state developing under doping.

Authors: Chikara Shalinee; Fabbris Gilberto; Qi Tongfei, Terzic Jasminka, Cao Gang, Haskel Daniel Argonne National Laboratory, X-ray Science Division

STUDYING EXOTIC NUCLEI USING A NEW FAST BETA-DECAY TAGGING SYSTEM AT ARGONNE

Nuclei with the same number of protons and neutrons are of special interest in nuclear physics. In such nuclei, the neutrons and protons occupy the same orbitals, leading to the amplification of structure effects. Odd-odd, self-conjugate nuclei exhibit distinctly different characteristics when compared with neighboring nuclei and are therefore a particular focus for experimental and theoretical efforts. Several theoretical frameworks have been developed in an attempt to probe the structure of these nuclei (e.g. [1,2,3]), and a much higher density of low-lying energy levels have been predicted than currently observed. Experimental studies of exotic nuclei present a number of challenges as production cross-sections are typically very low compared with contaminant species. A new experimental system, designed to obtain structure information for exotic nuclei close to the N=Z line, has been recently developed at the Argonne ATLAS facility. The system provides extremely high levels of selectivity on exotic nuclei of interest by taking advantage of their characteristically fast beta decays.

Authors: David, Helena M
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THE IMPACT OF PSEUDOMONAS FLUORESCENS STRAINS ON ASPEN GROWTH DURING PHOSPHORUS AND NITROGEN LIMITATION

Symbiotic relationships influence survival and productivity in forest ecosystems and consequently affect ecosystem carbon-nutrient cycling. In addition to fungal associations, some bacteria can also play a major role in plant nutrient uptake and protection from pathogens. These bacteria are classified as mycorrhizal helper bacteria (MHB) based on their ability to promote mycorrhizal formation and enhance plant productivity in low nutrient soils. To better understand the role of these MHB-plant associations, we examined the impact of several *P. fluorescens* strains (WH6, SBW-25, Pf0-1, and PF-5) on the in vitro growth of aspen seedlings at control versus low concentrations of nitrogen and phosphorous. Control and nutrient limited seedlings were grown with and without the MHB on vertical petri-plates in controlled environmental conditions. Growth rate and morphology were assessed as primary indicators of plant health and the number of leaves, plant shoot height, root length and root structure such as branching pattern and rootlets were evaluated weekly. Our results show nutrient limitation reduces the number of leaves, but increase root length and branching structure. The number of seedling rootlets decreased significantly during phosphorus stress, but increased during nitrogen stress. The effects of MHB colonization on plant growth and root morphology were found to be strain dependent. An increase in the number of leaves was observed in control seedlings colonized with all bacterial strains. Similar strain dependent effects were also observed under nutrient limiting conditions. More complex root branching was observed for seedlings under phosphorus and nitrogen stress in comparison to the control seedlings when plants were colonized by Pf0-1 and SBW-25. Further understanding of nutrient limitation effects is expected to increase our insight into community structure and carbon cycling in terrestrial ecosystems.

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MODELING CENTRAL CARBON CORE METABOLISM IN MICROBIAL LIFE

Hundreds of microbial genomes are now being sequenced every day, demanding the analysis of a wide variety of microbes that may be utilized in multiple medical and industrial applications. Metabolic models are becoming widely popular and useful for the high-throughput prediction of microbial phenotypes and behavior. The Model SEED framework (Henry, DeJongh et al. 2010) provides a means for automated constructing of genome-scale metabolic models using high quality annotations from SEED subsystems (Aziz, Bartels et al. 2008). One of the common problems identified in draft models generated by the Model SEED is a lack in accuracy of pathways predicted for electron transport and ATP production.

Central carbon pathways, electron transport chain (ETC), and fermentation pathways play an essential role in accurate metabolic modeling, and these pathways depend on environmental factors such as carbon source/electron donor, presence of oxygen or other anaerobic electron acceptors and the fermentation capability of the organism. Unlike eukaryotic organisms, bacteria ETC are highly diverse and complex, being categorized into obligate aerobic, obligate anaerobic, photosynthetic and facultative. As a result, the terminal electron acceptors range from organic compounds such as dimethyl sulfoxide (DMSO), trimethyl aminoxide (TMAO) numerous inorganic compounds such as nitrate, nitrite, sulphate, iron, etc. To overcome this problem, we developed tools to build high-quality core models based on well-studied, phylogenetically diverse model organisms, including *Escherichia coli*, *Bacillus subtilis*, *Pseudomonas aeruginosa*, *Clostridium acetobutylicum* and *Paracoccus denitrificans*. High quality core models may then be integrated into genome scale metabolic models, significantly improving the accuracy of energy metabolism pathways. We applied these tools to produce core metabolic models for over

8000 genomes, designed to be accurate depictions of central carbon metabolism, ETC, and energy production for microbial organisms. Building and analyzing core models on almost every single sequenced bacterium helps to understand their metabolism on diverse environments and the metabolic variation in relationship to the phylogenetic distances. Phylogenetic tree analyses based on the metabolic models of these organisms were able to depict evolution of central carbon pathways, fermentation pathways and ETCs. These analyses help to identify important metabolic shifts occurred during evolution, inconsistencies in genome annotation and gaps in the metabolic network of these pathways.

All tools developed for reconstruction, visualization, and analysis of core models were built into the DOE Systems Biology Knowledgebase (<http://kbase.science.energy.gov>), where they are available for use by the scientific community. We will highlight these tools in the context of our core model analysis.

Authors: Edirisinghe, Janaka N; Conrad, Neal; Xia, Fangfang; Overbeek, Ross; Henry, Christopher S
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PAIR DISTRIBUTION FUNCTION TECHNIQUES FOR THE STRUCTURAL CHARACTERIZATION OF SOLAR FUELS CATALYSTS AND A NEW ALGORITHM FOR AUTOMATIC MODEL FITTING: PDFIT

Rising urgency of transitioning from a fossil fuel-based to a renewable energy-based economy pushes research towards making solar energy cheaper and more readily available. To effectively utilize and store solar energy, photons coming from the sun need to be converted into electricity via photovoltaics technology or directly into fuel via artificial photosynthesis.

Hydrogen has a very high energy density per unit mass and its combustion is carbon neutral, therefore it is a very good candidate as clean fuel for many applications; furthermore Hydrogen is a virtually inexhaustible source of energy since it can be extracted from water via photolysis enhanced by the use of water-splitting catalysts. Amorphous thin-film metal-oxide water-splitting catalysts are of growing, wide-spread interest for development as catalysts for applications in solar fuels photochemical device applications, thanks to their robustness, benign operating conditions for catalysis, self-healing properties, and elemental abundance.

Authors: Fazi, Diego; Tiede, Dave, M
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HIGH PRESSURE GAS-FILLED CAVITIES FOR USE IN A MUON COOLING CHANNEL

A high pressure hydrogen gas-filled RF (HPRF) cavity can operate in the multi-Tesla magnetic fields required for a muon accelerator cooling channel. A beam test was performed at the Fermilab MuCool Test Area by sending a 400 MeV proton beam through an 805 MHz cavity and quantifying the effects of the resulting plasma within the cavity. The resulting energy loss per electron-ion pair produced has been measured at $10E-18$ to $10E-16$ J every RF cycle. Doping the hydrogen gas with oxygen greatly decreases the lifetime of an electron, thereby improving the performance of the HPRF cavity. Electron lifetimes as short as 1 ns have been measured. The recombination rate of positive and negative ions in the cavity has been measured on the order of $10E-8$ cm³/s. Extrapolation in both gas pressure and beam intensity are required to obtain Muon Collider parameters, however the results indicate HPRF cavities can be used in a muon accelerator cooling channel.

Authors: Freemire, Ben, T.; Tollestrup, Alvin, V.; Yonehara, Katsuya; Chung, Moses; Torun, Yagmur
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SYNCHROTRON X-RAY STUDIES OF THIN FILM SOLID OXIDE FUEL CELL CATHODES

Solid oxide fuel cells (SOFCs) are a scalable, fuel-flexible, and efficient technology for energy conversion. However, several materials design and efficiency challenges still limit their performance. In particular, the oxygen reduction reaction at the cathode is known to be a rate-limiting step in the energy conversion process. To improve SOFC performance, it is crucial to gain a better fundamental understanding of the reduction reaction mechanism and its relation to changes in the cathode structure and composition during cell operation.

Synchrotron measurements at the Advanced Photon Source are providing unique insight into the oxygen reduction reaction. One common cathode material for SOFCs is strontium- and cobalt-doped lanthanum ferrite (LSCF), which possesses excellent mixed ionic and electronic conductivity. In the work I will discuss, the oxygen exchange reaction of LSCF was investigated using pseudo half-cells consisting of a thin film of LSCF grown by pulsed laser deposition on a yttria-stabilized zirconia (YSZ) substrate, with a gadolinium-doped ceria (GDC) buffer layer. An important variable in the performance of LSCF is the oxygen vacancy concentration and its response to changes in SOFC operating conditions. We have determined changes in the oxygen vacancy concentration of thin film cathodes in response to electrochemical bias by using synchrotron x-ray diffraction to measure changes in the film's lattice parameter, which increases with increasing oxygen vacancy concentration. The characteristic time constants of the changes in oxygen vacancy concentration and current across the cell were used to determine activation energies and surface exchange rates for oxygen transport through the cathode during operation.

Authors: Hopper, E. Mitchell; Ingram, Brian J.; Chang, Kee-Chul; Baldo, Peter M.; You, Hoydoo; Eastman, Jeffrey A.; Fuoss, Paul. H
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DESIGNING SOLUBLE PRECURSORS FOR THIN-FILM PHOTOVOLTAICS

We first report a new platform for design of soluble precursors for CuInSe₂ (CIS), Cu(In_{1-x}Ga_x)Se₂ (CIGS), and Cu₂ZnSn(S,Se)₄ (CZTS) phases for thin-film photovoltaics. To form these complex phases, we used colloidal nanocrystals (NCs) with metal chalcogenide complexes (MCCs) as surface ligands. The MCC ligands both provided colloidal stability and represented essential components of target phase. For instance, a mixture of Cu₂Se and ZnS NCs, both capped with (NH₄)₄Sn₂S₆ or (NH₄)₄Sn₂Se₆ ligands was used for solution deposition of CZTS films. These precursors can be readily transformed into continuous films of PV relevant semiconductors in a very atom-economic way, with minimal weight loss and volume contraction. We then performed comparative mechanistic study on the formation kinetics of crystalline CZTS thin-films via depositing and annealing various liquid-phase precursors. We find out that dimensionality of precursors largely determines the kinetics of solid-state reactions: molecular species can be more conveniently transformed into CZTS given low annealing temperature/short annealing time, while bulky precursors lead to the formation of larger CZTS crystallites at later stage. Besides, when colloidal NCs are used as precursor components, their surface chemistry and the solvents both influence the sintering kinetics. Lastly, we have demonstrated for the first time that solid-state phase transition can dramatically enhance crystallization of CZTS under mild heat treatment, thus providing a new strategy towards design of soluble precursors for fabrication of CZTS and other inorganic phases. Apart from these, we have synthesized monodispersed Cu₂Se and Cu₂Te nanocrystals for the first time and found that their plasmonic features can be easily tuned by adding oxidants (such as oxygen) and reductants (such as hydride) or by changing the dielectric environments (such as solvents or surface ligands). These nanocrystals show interesting plasmonic features due to the propensity to oxidation of Cu⁺ ions that creates excess holes located at the top of valence bands. Our results are significant not only in helping further understand surface plasmon of nanocrystals, but also in potential applications such as solar cells and photothermal therapy.

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HAFNIUM CLUSTER CHEMISTRY: TOWARD SCALABLE MATERIALS DESIGN, DISCOVERY, AND CREATION

Novel inorganic compounds are currently obtained by 'cook-and-look' practices, with no real attempt to design the synthetic routes. As the demand for complex materials needed in future technologies increases, a more sophisticated approach is required for materials engineering. Our approach to this wide-reaching problem is based on the synthon, a concept that has been in common use in organic synthesis of decades. Synthons are the synthetic building blocks used to build up larger organic molecules and infinite structures. They can be thought of as molecular fragments, which are intermediary between atoms and bulk materials. To find suitable models to begin realizing this approach for inorganic materials, we turned to metal-oxo-clusters which form in aqueous solutions. These have interesting architectures which can often be structurally related to the corresponding metal oxides. ZrO₂ and HfO₂ are important materials in microelectronics,[1] ceramics[2] and catalysis.[3] As small highly charged cations, Zr⁴⁺ and Hf⁴⁺ undergo hydrolysis easily in aqueous solutions. We chose to study the formation of Hf⁴⁺ clusters in sulfuric acid solutions, since the sulfate anion can bridge metal centers promoting cluster formation. From these solutions come rather unusual polynuclear metal-oxo-hydroxo clusters which then crystallize, enabling their structure determination. But despite their structural diversity, only four such structures were found: a dimer,[4] a planar hexamer,[5] a 17-mer[6] and an 18-mer.[7] By identifying new clusters and studying their formation in solution, we hope to gain some understanding of the mechanisms of cluster formation and the relationships between clusters and bulk materials.

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Authors: Kalaji, Ali, Soderholdm, Lynda
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PROBING CHEMICAL REACTIVITY AND STRUCTURAL DEFECTS IN NIOBIUM CAVITIES: IMPROVING THE NEXT GENERATION OF PARTICLE ACCELERATOR

Niobium is the preferred material used for Superconducting Radio Frequency (SRF) cavities in particle accelerators. Chemical and structural defects formed on the cavity surface during preparation can significantly reduce cavity performance, in some cases rendering them useless under high-field gradients. This work is motivated in part by the observation that baking the cavity at modest processing temperatures (100-400 oC) can lead to improved cavity performance. We use a number of surface science techniques to better understand the role these defects have on the chemical reactivity and diffusion kinetics of common cavity contaminants (oxygen, hydrogen, water, nitrogen). X-ray photoelectron spectroscopy (XPS) shows the oxidation state of a polycrystalline sample cut directly from an SRF cavity changes with sputtering and thermal heat treatments. Scanning electron microscopy (SEM) and atomic force microscopy (AFM) images of this sample reveal that despite extensive chemical and mechanical polishing, a number of surface defects and weld pits exist on the surface. The role of the local surface

environment on chemical reactivity (including step edges, dislocations, point defects, and grain boundaries) is investigated by scanning tunneling microscopy (STM). A new UHV instrument was built to allow samples to be heated to temperatures >1800o C before transfer into the STM imaging chamber. Single-crystal niobium substrates are used to study the influence of crystalline structure, terrace\ shape and size, step edges, and surface dislocations on the adsorption, dissolution, and formation of surface oxides. We observe that initial crystal orientation significantly affects the formation of surface oxide structures; the NbO-(111) surface does not present any long-range order despite extensive high-temperature heating, while the NbO-(100) easily forms highly-organized (nx1) ladder structures (Figure 1). We will discuss the stability and conversion of the NbO-(100) oxide features upon thermal annealing with and without the addition of gas-phase oxygen and nitrogen, with particular focus on dissolution from the surface to the bulk upon low-temperature annealing of the substrate. Further, we discuss the role of niobium oxide as a capping layer that influences chemical reactivity at the gas-surface interface.

Authors: Kautz, Natalie, A; Gibson, Kevin, D; Nakayama, Miki; Wang, Tuo; Sibener, Steven, J.
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KIRKPATRICK-BAEZ MIRRORS TO FOCUS HARD X-RAYS IN 2-D ARE FABRICATED, TESTED, AND INSTALLED AT THE ADVANCED PHOTON SOURCE

We report on the design of the Kirkpatrick-Baez (K-B) mirrors mounting system, mirrors fabrication, and performance of the focus spot. The K-B mirror assembly is fully developed by the APS optics group and was designed for installation at 8-BM beamline. The two elliptical mirrors are arranged in sequential K-B optics. The mirrors are coated with Platinum (Pt) material on Si substrate. The vertical focusing mirror of 80 mm length with focal length of 255 mm and horizontal focusing mirror of 60 mm length with focal length of 155 mm. Magnetron sputtering deposition techniques was used to achieve the elliptical shape on the flat Si substrates. Metrology measurements showed that the figure errors for the 80 mm and 60 mm long mirror are 0.61 nm and 0.33 nm. A doubly focused 1.3(vertical) μm x 1.2(horizontal) μm with monochromatic beam at 18keV was measured. The beamline layout, the techniques for characterizing the beam focal spot and performance of the mirrors are discussed.

Authors: Naresh Kujala; Shashidhara Marathe; Deming Shu; Bing Shi; Jun Qian; Lydia Finney; Chris Jacobsen; Albert Macrander; and Lahsen Assoufid
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TA0.3Ti0.7O2 ELECTROCATALYST SUPPORTS EXHIBIT EXCEPTIONAL ELECTROCHEMICAL STABILITY

Ta modified TiO₂ was synthesized using a sol-gel procedure and evaluated for use as an electrocatalyst support. Platinum nanoparticles were deposited on this support via the incipient wetness method. X-ray diffraction (XRD), transmission electron microscopy (TEM), X-ray energy dispersive spectroscopy (XEDS), X-ray photoelectron spectroscopy (XPS) and nitrogen desorption were used to investigate their microstructure. The capacitance of the Ta_{0.3}Ti_{0.7}O₂ support changed by only 12% whereas the pseudocapacitance of a carbon benchmark changed by over 100% over 10,000 potential cycles under identical test conditions. The stability of the catalysts were evaluated by monitoring the evolution of the electrochemical surface area (ECSA) under potential cycling, and the loss in ECSA of Pt/Ta_{0.3}Ti_{0.7}O₂ was found to be 35% compared to 46% for Pt/C over 10,000 load cycles. Pt/Ta_{0.3}Ti_{0.7}O₂ showed relatively good performance: the ECSA of this electrocatalyst was 41 m²/g, the mass activity and area-specific activities for the oxygen reduction reaction (ORR) were 62 mA/mgPt and 151 $\mu\text{A}/\text{cm}^2\text{Pt}$, respectively. Koutecky-Levich analysis carried out to evaluate ORR kinetics revealed that both Pt/Ta_{0.3}Ti_{0.7}O₂ and Pt/C demonstrated similar ORR mechanisms. Based on these results, we propose that Ta_{0.3}Ti_{0.7}O₂ shows outstanding promise as a corrosion-resistant alternative to carbon as an electrocatalyst support in polymer electrolyte fuel cells.

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PRECAM, THE PRECURSOR TO THE DARK ENERGY SURVEY

We are interested in assigning a pre-specified number of nodes as leaders in order to minimize the mean-square deviation from consensus in stochastically forced networks. This problem arises in several applications including control of vehicular formations and localization in sensor networks. For networks with leaders subject to noise, we show that the Boolean constraints (a node is either a leader or it is not) are the only source of nonconvexity. By relaxing these constraints to their convex hull we obtain a lower bound on the global optimal value. We also use a simple but efficient greedy algorithm to identify leaders and to compute an upper bound. For networks with leaders that perfectly follow their desired trajectories, we identify an additional source of nonconvexity in the form of a rank constraint. Removal of the rank constraint and relaxation of the Boolean constraints yields a semidefinite program for which we develop a customized algorithm well-suited for large networks. Several examples ranging from regular lattices to random graphs are provided to illustrate the effectiveness of the developed algorithms.

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URANYL(VI) AND PLUTONYL(VI) COORDINATION AND DYNAMICS IN A TASK-SPECIFIC IONIC LIQUID

Ionic liquids (ILs) are a unique class of solvents with potential applications in advanced separation technologies relevant to the nuclear industry. ILs are salts with low melting points and a wide range of tunable physical properties, such as viscosity, hydrophobicity, conductivity, and liquidus range. ILs have negligible vapor pressure, are often non-flammable, and can have high thermal stability and a wide electrochemical window, making them attractive for use in separations processes relevant to the nuclear industry. Metal salts generally have a low solubility in ILs; however, by incorporating new functional groups into the IL cation or anion that promote complexation with the metal, the solubility can be greatly increased. One such task-specific ionic liquid (TSIL) is 1-carboxy-N,N,N-trimethylmethanaminium bis(trifluoromethylsulfonyl)imide ([Hbet][Tf₂N]) [Nockemann et al., J. Phys. Chem. B 2006, 110, 20978-20992]. Water, which is detrimental for electrochemical separations, is a common impurity in ILs and can coordinate with actinyl cations, particularly in ILs containing only weakly coordinating components. Understanding the behavior of actinides in TSIL/water mixtures on a molecular level is vital for designing improved separations processes. Classical molecular dynamics simulations of uranyl(VI) and plutonyl(VI) in 1-ethyl,3-methylimidazolium bis(trifluoromethylsulfonyl)amide ([EMIM][Tf₂N]) with de-protonated Hbet (betaine) and water have been performed to understand the coordination and dynamics of the actinyl cations. We find that the betaine is a much stronger ligand than water and prefers to coordinate the metal in a bidentate manner. When very little betaine is present, all of it coordinates the actinide, with the remainder of first solvation shell filled by water. As the amount of betaine coordinated to the actinide increases, the diffusion coefficient of the actinyl cation decreases. The betaine ligand is able to bridge between two metal centers, resulting in dimeric complexes with actinide-actinide distances of approximately 5 Å. Potential of mean force simulations show that these structures are stable, with relative free energies of up to -40 kJ/mol. The crystal structure for uranyl betaine shows that the betaine bridges between two uranium atoms to form dimeric complexes similar to those found in our simulations [Nockemann et al, Inorg. Chem. 2010, 49, 3351-3360].

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DEVELOPMENT OF NANOSILICON-POLYANILINE CAPSULES FOR RENEWABLE ENERGY APPLICATION

We are developing a novel nanostructured organic/inorganic composite material for photovoltaic and renewable energy applications. The material integrates nanosilicon with conducting polymer in a closely coupled configuration: a polyaniline (PANI) nanocapsule with a highly luminescent core consisting of 2.9 nm silicon nanoparticles. Both silicon, a biocompatible material, and PANI are known components of solar cells, but their combination extends the absorption range to cover nearly the entire solar spectrum. PANI-nanoparticle capsules appear to be an effective dual sensitizer material due to PANI's good electric transport and fast resonance tunneling between the monodispersed Si nanoparticles. The nanoscale capsule structure affords more efficient charge separation and removal. The nanocapsules are characterized using scanning electron microscopy (SEM), X-ray photoelectron spectroscopy (XPS), atomic force microscopy (AFM), energy dispersive spectroscopy (EDS) and bright and dark field optical microscopy. Charge transport is analyzed in terms of material bandgaps and electron affinity and the electrochromatic property of PANI.

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ATOMIC LAYER DEPOSITION OF IN₂S₃ VIA A NOVEL INDIUM AMIDINATE PRECURSOR

Atomic layer deposition (ALD) allows for unique control over semiconductor, insulator, and metal formation.¹ Alternating between vapor pulses of different chemical precursors (say an indium source and a sulfur source) grows these materials one atomic layer at a time. Our eventual goal is to utilize this technique to create thin films of V_{0.25}In_{1.75}S₃ for intermediate band solar cells (IBSC), but our first step is to create In₂S₃ thin films by ALD. While this process has already been reported in the literature using indium acetylacetonate (In(acac)₃) as a precursor,² this compound could decompose and leave oxygen (and carbon) impurities in our films.³ An IBSC requires precise doping to achieve increased solar absorption, so in the work presented here we have explored a new indium precursor for cleaner, and novel ALD. Indium (III) N,N'-diisopropylacetamidinate (InAm) contains no oxygen atoms, has a greater thermal stability than In(acac)₃, and was found to be highly reactive. Using this novel precursor resulted in comparable growth rates and comparable film quality versus In(acac)₃, but without oxygen impurities. Further optimization will lead to improved electronic properties required for our devices.

Authors: McCarthy, Robert F.; Weimer, Matthew; Pellin, Michael J.; Hock, Adam S.; Martinson, Alex B. F.
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ATOMIC LAYER DEPOSITION OF METAL SULFIDES FOR HIGH PERFORMANCE LITHIUM BATTERIES

Electrical storage devices are essential for the wide-scale implementation of renewable energy sources such as solar and wind energy. Lithium-ion batteries (LIBs) are attractive in this regard, but many challenges remain. One of the main issues lies in the limited capacities of the existing electrodes: the graphite anode and the lithium metal oxide. In this context, great research effort

is being directed towards new electrode materials with the hope of dramatically increasing the LIB energy density. Among the candidate materials, metal sulfides represent a very promising class and can serve as the anode, cathode, or the solid electrolyte. As a relatively new area, however, metal sulfides remain largely unexplored for LIBs. In our current research within CEES, we are using atomic layer deposition (ALD) for synthesizing metal sulfide thin films and nanomaterials for LIBs. In contrast to conventional material fabrication processes, ALD provides atomic-level control over material growth, unrivalled uniformity and conformality of deposited films, and highly flexible tunability in material composition and crystallinity. To date, we have synthesized gallium sulfide (GaSx), copper sulfide (Cu2S), lithium sulfide (LiS-x), and lithium gallium sulfide (LiGaxSy) materials. Furthermore, through depositing these metal sulfides on nanostructured templates such as carbon nanotubes and graphene, we have developed many nanostructured composites that demonstrate excellent electrochemical performance during charge-discharge cycling of LIBs. For instance, GaSx, Cu2S, and their nanostructured composites prepared by ALD exhibited long-term stability (>1000 cycles) as anodes. In addition, LiSx is one of the most promising cathode materials, providing a capacity 5x higher than current lithium metal oxides. The ALD of LiSx might provide a viable route to high performance lithium-sulfur batteries. In this presentation, I will describe our unique ALD synthesis routes for the metal sulfides and also demonstrate their exceptional electrochemical performance.

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DYNAMIC OF RU-CL SOLVENT EXCHANGE AND ITS ROLE IN CATALYTIC WATER OXIDATION BY [RU(BPY)(TRY)CL]+ CATALYST

[Ru(II)(bpy)(tpy)Cl]+ (bpy = 2,2'-bipyridine, tpy = 2,2'; 6',2''-terpyridine) complex has been demonstrated to work as water oxidation catalyst. However, it does not have -H2O ligand to allow for proton coupled electron transfer and formation of activated Ru=O species. NMR was previously used to assess the dynamic of Ru-Cl exchange but it has limitation that only diamagnetic Ru(II) species can be analyzed. Here we show how Cl K-edge XANES can be effectively used to study Ru-Cl bond dissociation. We show that in agreement with chemical intuition Ru-Cl exchange rate is significantly impeded by oxidation of RuII to RuIII (no quantifiable exchange was observed within 4 hours). Ru L-edge and K-edge XANES and EPR also show that [Ru(II)(bpy)(tpy)Cl]+ complex does not oxidize past RuIII state by ammonium cerium(IV) nitrate in nitric acid at pH 1 while [Ru(II)(bpy)(tpy)H2O]+ complex partially converts to [Ru(IV)=O(bpy)(tpy)]2+. Taking all above results into account [Ru(II)(bpy)(tpy)Cl]+ should not be a water oxidation catalysts. Its catalytic activity is likely due to effect of prior acetonitrile dissolution (which facilitates Cl exchange (Thummel, 2012) or due to partial removal of organic ligand via ligand oxidation in the presence of significant excess of Ce(IV) to provide coordination center for H2O binding.

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COEXISTENCE OF TWO DIFFUSION MECHANISMS: W ON W(100)

Fabrication of nano- electronic devices, requires greater understanding of the surface phenomena. Changing the diffusion mechanisms just by changing the temperature gives tremendous advantage in fabrication of single atom devices. In future applications, the occurrence of two diffusion mechanisms: adatom jump and adatom exchange, in one system, could give a possibility for transporting the adatom into designated area via jump and then burying it in the first layer of the surface by using the exchange mechanism. However, even though the occurrence of the two diffusion mechanisms has been postulated over the years, it has yet to be shown experimentally. Here we demonstrate a first experimental proof for the occurrence of those two mechanisms for W on W(100) system. We show that while the adatom diffuses via the exchange mechanism, it is possible to trigger the additional diffusion mechanism – the jump, just by increasing the temperature. In our analysis we provide the value of the activation energy for the diffusion of W on W(100) via the exchange mechanism and the estimated value for activation energy for diffusion via jump. The diffusion parameters were calculated from direct measurements of the mean square displacement of diffusing adatom. The position of the adatom was determined with Field Ion Microscope which allows imaging the surface with atomic scale resolution. The experiments were conducted in ultra-high vacuum conditions. The diffusion mechanisms were deduced from comparison the arrangement of positions of diffusing W adatom with the arrangement of the adsorption sites obtained from = deposition W and Rh adatoms on W(100) surface.

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A LEARNING ALGORITHM FOR SPACE MAPPING AND SEARCHING USING ADAPTIVE MESH REFINEMENT

In a complex self-organizing system, small changes in the system's basic constituents can result in different emergent macrostructures or macro-behaviors. In chemical engineering and material science, such spontaneously self-assembling systems, using polymers, nano- or colloidal scale particles, DNA, or other precursors, are an attractive way to create fine-scale precisely engineered materials. Changes to the constituents or inputs can be described by a set of parameters and different contiguous regions in this parameter space corresponds to the self-assembly of different ordered states. Since these ordered states are emergent, often experiment, not analysis, is necessary to discover what happens where. Using computational or physical experiments, these contiguous regions can be discovered and mapped by queries at points in the parameter space to

construct a phase diagram. However, queries can be costly in terms of resources or time. In general, one would like to learn the most about the phase diagram of a space for the fewest total number of queries. Here we introduce a learning algorithm for issuing queries to map and search a two-dimensional parameter space. Using a method inspired by the adaptive mesh refinement method, the algorithm iteratively issues batches of queries, to be executed in parallel, based on what has been learned from previous iterations. By adjusting the search criteria of the algorithm, different types of searches (e.g. a uniform search, exploring boundaries, sampling all regions equally) can be flexibly implemented. We show that this method will search the whole space in the limit of infinite queries while preferentially targeting certain features of space. Using numerical examples, we show how this algorithm can discover new regions and map boundaries more accurately than a uniform distributed set of query points.

Authors: Phillips, Carolyn, L.

Argonne National Laboratory, Mathematics and Computer Science Division

ORBITAL ANGULAR MOMENTUM OF PHOTONS AND HIGH-HARMONIC GENERATION

Light beams can transport spin (SAM) and orbital (OAM) angular momentum, related to its polarization and spatial structure respectively. For infrared (IR) and optical wavelengths, light beams with well-defined OAM can be generated using diffractive masks to imprint a phase twist in the wavefront. Although in the x-ray regime similar methods can be found, high-quality diffractive masks are not so easy to produce.

In our theoretical proposal we show that x-ray vortices can be created through high-harmonic generation (HHG). HHG is an extreme nonlinear process in which an electron is removed from an atom by an IR laser to be subsequently driven back to the parent ion, during the same laser field oscillation. Upon recollision the electron recombines with the parent ion emitting ultrashort x-ray flashes, at the attosecond timescale (10^{-18} s). Using HHG we have shown that it is possible to generate helical pulses in the x-ray regime that inherit the temporal and spatial coherence of the IR laser. The combination of OAM with the spatio-temporal characteristics of HHG leads also to the prediction of twisted attosecond pulse trains. Our work merges two distant topics in Optical Science with promising perspectives for non-linear and attosecond physics, optical and quantum communications, ultrafast micromanipulation, microscopy, and spectroscopy, among others.

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TOWARDS OPTIMAL WORKFLOW TO SUPPORT MASSIVELY PARALLEL IMPLICIT ADAPTIVE COMPUTATIONAL FLUID DYNAMICS SIMULATIONS ON COMPLEX GEOMETRIES

The development of massively parallel computation, along with scalable numerical methods, provides the capacity to perform simulation on a time scale that has enabled incredible scientific breakthroughs in computational mechanics in the last decade. However, the efficient exploitation of these ever growing computational power requires both current and new key ingredients to be carefully coupled in order to compress further the time-to-solution for challenging problems in science and engineering. In particular, with the upcoming emergence of exascale machines, not only the size of the problem and its associated computation time will have to be taken into account, but also the time to set up the case and to process the resulting ever-larger data in order to perform any assessment of the insight in a reasonable time.

Authors: Rasquin, Michel; Smith, Cameron; Chitale, Kedar; Seol, Seegyoung; Matthews, Benjamin; Sahni, Onkar; Shephard, Mark; Jansen, Kenneth

Argonne National Laboratory, Leadership and Computing Facility

DEVELOPMENT OF A PROTOTYPE CALIBRATION SYSTEM FOR THE LBNE PHOTON DETECTION SYSTEM

The Long-Baseline Neutrino Experiment (LBNE) is a broad scientific program being developed in the United States with strong international participation. The primary goal of LBNE is to reach an unprecedented sensitivity and precision for addressing the questions related to neutrino mass hierarchy, CP violation in neutrino sector and values of neutrino mixing parameters including precision measurement of θ_{13} . In order to achieve these goals, it will require an intense neutrino beam produced at Fermi National Accelerator Laboratory (Fermilab), a large neutrino detector located at the Homestake site in South Dakota, nearly 1300 km downstream from the neutrino source. The high-intensity neutrino beam will allow LBNE to make high precision measurements with neutrinos and anti-neutrinos separately. This is crucial for the measurement of charge-parity violation, leading to the ability to understand matter-antimatter asymmetry and resulting dominance of matter in the universe. To meet the scientific and technical objectives, LBNE will use a 10^{34} kton Liquid Argon Time Projection Chamber (LArTPC) as the far detector at Homestake site in South Dakota. Neutrino interaction in LAr result in charged particles producing ionization and scintillation light signals. By detecting scintillation light we aim to efficiently separate neutrino events from background. In this talk, I will describe the ongoing work at Argonne High Energy Physics Division on the development of a new prototype for calibration of the photon detection system of the LBNE detector. Our prototype system uses the light from an LED (or a laser) being fed through the Liquid Argon volume using optical fibers and received by silicon photo-multiplier (SiPM) photo-sensor. Details of the calibration system and planned tests with LAr test stand at Fermilab will be covered in this talk.

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STABILIZING CU₂S PHOTOVOLTAICS VIA ULTRATHIN ALD BARRIER LAYERS

Thin film photovoltaic (PV) technologies based on Cu(In,Ga)Se₂ (GIGS) and CdTe combine moderate efficiencies with low cost. However, expanding to terawatt production brings concerns about material sustainability and hence, future costs. As such, there is a clear and present need for an alternative absorber, whose constituent elements are earth abundant, environmentally benign, and therefore, exhibit even lower projected materials and recycling costs. Cu₂S was identified decades ago as a potential PV absorber due to its exceptional combination of these desired properties, as well as a suitable band gap of 1.2 eV, an absorption coefficient >10⁴, p-type conductivity, and a theoretical solar conversion efficiency of 28%.¹ Despite such promising attributes, a major hurdle preventing its practical utilization is the instability of the Cu₂S layer under working conditions. Early studies concluded that Cu-diffusion exacerbates the transformation of chalcocite (Cu₂S) to djurleite (Cu_{1.96}S), which alters the electronic properties and ultimately hinders its use as a PV material.¹ A second hurdle is an incongruity between the optical depth (LOD ≈ 1.3 μm) and minority carrier extraction length (LCE = ~150 nm). Nanostructuring Cu₂S thin films on high area scaffolds is one approach to decouple LOD and LCE and an area where ALD has thrived. We demonstrate high quality—phase pure, crystalline, and without cation impurities—Cu₂S thin films grown by ALD for which a change in electronic properties with time and environment have been evaluated. We find that exposure of pristine Cu₂S thin films to ambient conditions results in a rapid rise in conductivity due to heavy p-type doping (>10²⁰).² These results are corroborated with changes in the optical properties, surface composition, and crystalline phase of the Cu₂S thin films. Finally, we demonstrate that this deleterious pathway can be largely mitigated by ALD of ultrathin barrier layers (BL) at both the substrate/Cu₂S and Cu₂S/air interface.³

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AUTOMATED ¹⁸F LABELING OF SUCROSE FOR TRANSPORTER STUDIES IN PLANTS VIA AUTORADIOGRAPHY AND PET

Many plants sustain their growth and metabolism from sucrose exported from source leaves to carbon-importing sink tissues. In many dicot plants, evidence has been established that SUTs and specifically SUT1-type proteins function to import sucrose from the apoplast into the phloem cells.¹ The biological function of SUT1 in monocot plants such as maize was unclear until a maize *sut1* mutant (plant lacking SUT1) was isolated.¹ These plants had a severe reduction in plant growth and fitness compared to normal plants (wild type, WT). The ability of these mutants to transport sucrose was investigated with ¹⁴C-sucrose (- 0.157 MeV, t_{1/2} = 5.73x10³ yrs, universally labeled on all carbon atoms).² While informative, these radiotracer studies required destructive sampling in order to quantitate and visualize the location of the label by autoradiography, and were relatively slow, typically taking five days to obtain the data owing to time consuming and tedious sample preparation. As a sister experiment we have developed an automated method for the synthesis of F-18 (+ 0.635 keV, t_{1/2} = 110 min) labeled sucrose for use in the investigation of the local storage and transport of sucrose by SUTs in both wild-type and mutant maize via autoradiography and positron emission tomography (PET) imaging.

Authors: Rotsch, David; Brossard, Thomas; Ying, Waylon; Gaddam, Vikram; Swyers, Nathan; Harmata, Micheal; Cutler, Cathy; Robertson, David; Jurisson Silvia S; Braun, David
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RUBIDIUM-PROMOTED MOLYBDENUM CARBIDE CATALYSTS FOR MIXED ALCOHOL SYNTHESIS FROM SYNGAS

The catalytic conversion of synthesis gas derived from coal, natural gas or renewable biomass is a promising route to produce alternative energy carriers and chemical feedstock, and molybdenum carbide is potentially an effective catalyst for the reaction provided suitable promoters and activity gains are realized. The product distribution from CO hydrogenation over molybdenum carbide favors production of linear hydrocarbons via Fischer–Tropsch synthesis, whereas promotion of molybdenum carbide with alkali metals shifts the product distribution toward the production of mixed alcohols. In this study, nanometer-sized clusters of Mo₂C were supported on metal oxide supports and characterized by a variety of techniques, including X-ray absorption spectroscopy, electron microscopy and diffuse reflectance Fourier transform infrared spectroscopy of adsorbed CO. Steady-state isotopic transient kinetic analysis of the CO hydrogenation reaction over supported Mo₂C catalysts, with and without Rb promoter, was then used to elucidate fundamental kinetic parameters such as the intrinsic turnover frequency of the reaction and the coverage of surface intermediates leading to products. Results from isotopic transient kinetic analysis and spectroscopic characterization will be used to explain the observed influence of Rb promoter on the steady-state product distribution during CO hydrogenation.

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VISUALIZATION OF INDIVIDUAL DEFECT MOBILITY AND ANNIHILATION WITHIN CYLINDRICAL DIBLOCK COPOLYMER THIN FILMS ON NANOPATTERNED SUBSTRATES

Diblock copolymers are well-known examples of self-assembling systems, which become increasingly valuable for the fabrication of nanoscale structures. Thin films of these materials spontaneously form periodic microdomain structures of various symmetries. These self-assembled patterns have been used as nanolithographic masks to create patterns on substrates as well as templates for the further synthesis of metallic dots and nanowires. However, these applications require precise pattern registration and formation of long-range ordered nanostructures free from defects. Previous experimental studies of the defect mobility are limited, because of the poor time resolution and also the interacting strains from nearby defects. In this paper, we investigate the defect evolution of cylindrical PS-*b*-PMMA diblock copolymer thin films on nanopatterned substrates. Topographical templates allow us to align cylindrical domains macroscopically. In this way, we are able to isolate a pair of defects and to study their interactions and movements. Also, high-temperature time-lapse atomic force microscope (AFM) imaging enables us to probe real-time and real-space defect evolution directly.

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MESOSCALE MODELING OF ELECTROCHEMICAL CRYSTAL GROWTH FOR ADVANCED LITHIUM BATTERIES

A multiphysics phase-field model is being developed to simulate electrochemically driven microstructural evolution in advanced lithium batteries, considering multicomponent diffusion, stress equilibration, electrostatics and phase-stability. This work involves mesoscale simulations of oxide growth in Li-air batteries by modeling multicomponent mass transport, electrostatics, structural mechanics, and microstructure evolution. We are developing a new continuum scale model that considers large variations in constituent concentrations between phases, concurrent diffusion on substitution and interstitial lattices, and an original phase-field formulation. The study encompasses electrochemical crystal growth/dissolution as well as nanoscopic interfacial effects such as the electric double layer. In application to realistic systems, we seek to understand the factors influencing the performance, longevity and behavior of Li-air and similar advanced battery concepts. The model is derived from a thermodynamic description of the system as a functional of the concentration of ionic species (Li⁺, O₂⁻, A⁻ and e⁻) and a neutral solvent, the electrostatic potential, the local phase, and the local pressure. Working through the theory of irreversible processes, we can describe the electrochemical growth / dissolution process in a system of at least eight highly non-linear, coupled partial differential equations which must be solved numerically via the finite element method. We have selected the FEniCS package for this purpose, which is an open-source project developed by teams internationally and relies on the PETSc library for calculation, thus taking advantage of the latter's scalability and efficiency on computer clusters.

We have developed a phase-field formulation with a newly developed technique of calculating extreme concentration variations, on the order of 10²³ over a simulated interface width of 1 Å, in a numerically robust fashion [1]. The model is currently implemented in 1D in order to have fast turnaround in simulation results while the theory and implementation were being developed. Figure 1 shows a simulation of the ideally polarized electrode which naturally produces the electric interfacial double layer, a distinctly mesoscopic phenomenon and an important interfacial phenomenon for electrical energy storage systems.

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SUPERCONDUCTING VORTEX PINNING VIA NANOPATTERNING

Critical current (I_c), below which a superconductor can transmit electrical power without any energy loss, is limited essentially by the motion of vortices. The vortices can be pinned or trapped by nano-holes or magnetic dots created by nano fabrication. Here we report experimental investigation of the critical current of superconducting films with a novel nonuniform pinning array, a conformal array of nanoscale holes. We find that the conformal array of nanoscale holes provides a more significant critical current enhancement at high magnetic fields as compared to the widely studied triangular pinning array, which can be attributed to its arching effect that effectively prevents vortex channeling occurring in samples with a regular lattice of holes. In addition, we investigated vortex pinning effects of a ferromagnetic antidot array. Although there is no direct pinning enhancement by the pristine magnetic antidot array in perpendicular magnetic fields, we found that by applying an independently controllable in-plane magnetic field the magnetic antidot array can provide excellent vortex pinning, resulting in tunable critical current enhancement. Combining magnetic force microscopy imaging and micromagnetic simulation, we reveal that the tunable vortex pinning originates from the stray field generated by the magnetic antidot array in the presence of an in-plane magnetic field.

Author: Y. L. Wang, Z. L. Xiao, R. Divan, L. E. Ocola, G. W. Crabtree, and W. K. Kwok
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TRANSPORTED PDF MODELLING OF SPRAY COMBUSTION AT DIESEL ENGINE CONDITIONS

In diesel engines, cold fuel is introduced at high velocity to the cylinder containing hot, compressed air, and ignites resulting in a flame that is "lifted" from the fuel nozzle. The lift-off length, defined as the distance from the nozzle to the flame, has a strong bearing on emissions of NO_x and particulates, since it affects the amount of mixing of fuel and air prior to combustion. Advanced diesel engine combustion strategies therefore seek to control the lift-off length, and computational predictions of lift-off are needed to aid in design. However, at present, computational models for predicting the lift-off length are typically very basic. They assume that there are no turbulent fluctuations of the thermochemical state (e.g. temperature, chemical species mass fractions), i.e. that the fluid is well-mixed. However, due to the extreme nonlinearity of the chemical reaction rates, which are exponentially dependent on temperature, this approximation can lead to significant errors. The present work is aimed at improving this modelling by adopting the composition Probability Density Function (PDF) model, which solves for the turbulent fluctuations directly and in which the source term appears in closed form and can be treated exactly without approximation. The work represents among the first applications of this method to diesel spray combustion.

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ENHANCING CHEMICAL REACTIONS IN A CONFINED HYDROPHOBIC ENVIRONMENT: A NMR STUDY OF BENZENE HYDROXYLATION IN CARBON NANOTUBES

In situ solid state ¹³C NMR was employed for the first time to monitor the inside-outside distribution of molecules of different hydrophobicity. The results reveal that DWNT channels do not only discriminate hydrophobic benzene from hydrophilic acetic acid, but also expel the phenol out of CNTs where most acetic acid stays. As a result, the reaction equilibrium of benzene hydroxylation is shifted towards the product side leading to a significantly enhanced conversion. The study delivers a common concept of CNTs shifting the reaction equilibrium by selectively enriching hydrophobic molecules inside their channels and removal of hydrophilic molecules from the reaction system. Furthermore, the rich surface chemistry of graphene layers allows one to modulate the hydrophobicity of the inner wall and outer wall of CNTs through functionalization. This could lead to designing of efficient catalytic processes for a wider range of organic synthesis reactions involving molecules with different hydrophobicity in the reactants and products

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Argonne National Laboratory Postdoctoral Research and Career Symposium

ABSTRACTS

POSTER PRESENTATIONS



MAXIMIZING COMMUNICATION PERFORMANCE VIA SCALABLE, ROUTING-AWARE TASK MAPPING

The mapping of MPI processes to compute nodes in a supercomputer has a first-order impact on communication performance. Unfortunately, current practices for at-scale HPC do not use automatic mapping; instead using human experts for achieving good mapping. On the other hand, previously proposed techniques are either impractical (e.g., specific to niche topologies such as hypercubes [1], or non-scalable due to the use of mixed integer linear programming MILP as in IMR [2]). One key goal of my research is to achieve scalable, automatic mapping to maximize communication performance. My approach, Hierarchical Task Mapping (HTM) combines the use of (1) a divide-and-conquer heuristic to achieve scalability, and (2) an LP-based approach to evaluate possible mappings at the different levels of the hierarchy as well as to merge the partial solutions, to achieve high-quality mappings.

I applied my technique on one of the simulation applications called L-MESH. While HTM can run on any topology, I used the mesh networks for my experiments. I applied the technique on different mesh network sizes; 8x8, 16x16 and 32x32. I assumed the routing algorithm used in BlueGene/Q series of supercomputers where the communication can flow through any of the minimal-Manhattan paths from source to destination. I assume also that the tasks run in the virtual node mode in the BlueGene/Q where 16 tasks run on the 16 cores within one node. For example, for the case of 16,384 MPI tasks, they will be mapped to 1024 nodes (32x32 mesh). I compare HTM against the simple row major mapping and against the mappings based on the two space-filling curves (SFC); Moore and Hilbert. For the case of 4x4 mesh size where the IMR technique is feasible to use, I compared HTM against it. The metric for comparison is the maximum channel load (MCL) resulting from the each mapping.

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DIRECT NUMERICAL SIMULATION OF A HYDROGEN JET IN CROSS-FLOW

Enabling the next generation of low-emission, fuel-flexible gas turbine technology relies heavily on the design of rapid premixing sections, typically through the jet in cross flow (JICF) configuration. For highly reactive hydrogen or hydrogen-rich fuels, rapid mixing can result in unwanted autoignition in the premixing section leading to combustor damage. The autoignition process is a complex interaction between mixing and chemistry and is poorly understood. To address this issue, we use Argonne National Laboratory's Mira, the ALCF's 10-petaflops supercomputer, to investigate the complex dynamics of a diluted hydrogen jet issuing in a turbulent hot stream of air in a channel at different operating conditions. Highly nonlinear chemistry-turbulence coupling and huge scale separation complicate the dynamics, necessitating the use of an efficient high-order, method-based direct numerical simulation (DNS) code, such as Nek5000, and the computational power of Mira. In the first series of studies, we used the low Mach number solver based on the Nek5000 spectral element code to run large-scale simulations for two cross-flow temperatures (930 K and 950 K) and a channel friction Reynolds number of 180. In both cases, autoignition kernels initially form far downstream from the fuel nozzle creating propagating fronts which are convected out of the domain by the flow. Eventually radical buildup in the recirculation zone close to the nozzle exit results in a flame stabilized around the fuel jet. The DNS database is currently being interrogated to unravel the complex interaction of the local flow and mixing conditions with hydrogen chemistry leading to autoignition, the propagation characteristics of the flames around the kernels, and the flame stabilization mechanism. The chemical explosive mode analysis (CEMA) technique is employed to gain insight into the local reactivity of the fuel-air mixture, and identify regions of burned and unburned mixtures, local combustion mode, and flame stabilization mechanisms.

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SYNCHROTRON X-RAY SCANNING TUNNELING MICROSCOPY (SXSTM) AT THE ADVANCED PHOTON SOURCE

One fundamental challenge in surface science is the development of an analysis technique that can acquire chemical information with sub-nanometer resolution. The synchrotron x-ray scanning tunneling microscope (SXSTM) is a new lense-less microscope technique that is being developed to help meet this challenge. This technique will enable fundamentally new methods of materials characterization at the surface (catalysis, molecular transistor devices) and will potentially change our understanding of nano-scale phenomena.[1] The sub-nanometer scale chemical resolution is achieved by combining high brilliance x-ray radiation, supplied at the Advanced Photon Source, with scanning tunneling microscopy (STM). X-rays from the Advanced Photon Source provide the chemical information needed for this technique, and the scanning tunneling microscope provides the (atomic/electronic) spatial resolution. The SXSTM technique could lead to many exciting discoveries in materials science and could provide remarkable new insights into nano-devices and their behavior, for these devices will be the new building blocks of tomorrow's technology.

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Source, the Center for Nanoscale Materials, and the Electron Microscopy Center was supported by the U. S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under contract DE-AC02-06CH11357.

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PROCESS MODELING AND PERFORMANCE OPTIMIZATION OF CATALYTIC REACTORS

Process models are integral part of the performance monitoring system for many important industrial processes. Advanced process models, based on fundamental physical and chemical relationships, can help to optimize plant performance and increase revenue generation. In this presentation, I will discuss about our attempt to develop a process model for one of the world's largest catalytic reformer (CCR-Platformer) using first-principles approach. In our model, the reformer has been treated as a moving bed plug-flow reactor. The key aspects of model development will be discussed. Particular emphasis will be given on the deactivation of catalyst surface due to coke deposition and the regeneration of catalyst activity. We will also discuss about the role of solid state density functional theory (DFT) calculations in estimating model parameters where experimental results are not available. The model is tested by attempting to predict key operational parameters such as reaction temperature and concentration profiles of the reactor, heater duties, amount of coke on catalyst surface, and recycle gas composition for different feedstocks and operating conditions. Finally, the performance of our model will be compared with existing commercial models.

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DUALITY OF WEAK AND STRONG SCATTERER IN A LUTTINGER LIQUID COUPLED TO MASSLESS BOSONS

We study electronic transport in a Luttinger liquid with an embedded impurity, which is either a weak scatterer (WS) or a weak link (WL), when interacting electrons are coupled to one-dimensional massless bosons (e.g., acoustic phonons). We find that the duality relation between scaling dimensions (their product being equal to unity) of the electron backscattering in the WS and WL limits, established for the standard Luttinger liquid, holds in the presence of the additional coupling for an arbitrary fixed strength of boson scattering from the impurity. This means that at low temperatures such a system remains either an ideal insulator or an ideal metal, regardless of the scattering strength. On the other hand, when fermion and boson scattering from the impurity are correlated, the system has a rich phase diagram that includes a metal-insulator transition at some intermediate values of the scattering.

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SEARCHES FOR POSSIBLE T-ODD AND P-ODD SHORT RANGE INTERACTIONS USING POLARIZED NUCLEI AND NONMAGNETIC MASSES

Various theories predict the possible existence of T-odd and P-odd short-range forces between spin 1/2 fermions, proportional to $S \cdot r$ where S is the fermion spin and r is the separation between particles. We use ensembles of polarized nuclei obtained by Spin Exchange Optical Pumping and an unpolarized mass along with NMR technique to search for such a force over sub-mm ranges. We established an improved upperbound on the product $gsgpn$ of the scalar coupling to particles in the unpolarized mass and the pseudo-scalar coupling of polarized neutrons for force ranges from 10-4 to 10-2 m in high frequency resolution. This corresponds to a mass range of $2 \cdot 10^{-3}$ to $2 \cdot 10^{-5}$ eV for the exchange boson. Such techniques also have applications in navigation system gyroscopes due to their high precision.

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FIRST PRINCIPLES INVESTIGATION OF DUAL-FUNCTIONING ELECTROCATALYST/ELECTRODE MATERIALS FOR LI-O₂ BATTERIES

Recent experiments on Li-air batteries demonstrated that substantial enhancements may be achieved in energy efficiency and number of cycles when Li-Fe/Mn-oxides are used as dual-purpose electrocatalysts/electrode materials. The mechanisms of the improvements remain unknown. It is safe to say however, the characterization and control of the discharge ions and compounds (most notably Li and Li₂O) are key elements for the performance of metal oxides in batteries. Current work aims at establishing the thermodynamic conditions of Li or Li₂O removal from, and likewise re-incorporation into one such dual-functioning metal oxide Li₅FeO₄. In this sense, density functional theory is used as the principal method of investigation of the thermodynamic reactions in the given oxide. The calculation of total energies at various stages of Li/Li₂O removal and insertion allows us to associate the thermodynamic phases with equilibrium voltages and construct first principles phase diagrams. The energetic competition between Li and Li₂O removal is also revealed with the underlying electronic changes in the metal-oxide framework.

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IRON AND RHODIUM CATECHOL-CONTAINING POROUS ORGANIC POLYMERS: CHARACTERIZATION AND CATALYTIC REACTIVITY

Single-site, iron catecholate-containing porous organic polymers (POPs), Fe(II) and Fe(III), were prepared and characterized via ATR-FT-IR, Mössbauer, and in situ X-ray absorption spectroscopies. Fe(II) was utilized as a stable and remarkably active catalyst for the hydrosilylation of ketones and aldehydes. In some instances, catalyst loadings of 0.043 – 2.1 mol % [Fe] were sufficient for complete hydrosilylation of aldehydes and ketones within 15 min at room temperature. Exposure to air results in oxidation of the Fe(II) centers to Fe(III) deactivating the catalyst. Both batch and plug flow hydrogenation reactions were performed with these materials giving rise to two different catalytically active species. The catalysts can be recycled at least three times without a drop in catalytic activity, and are examples of immobilized homogeneous catalysts with no homogeneous analogue. Rhodium containing POPs were also prepared and characterized using ATR-FT-IR, NMR, and X-ray absorption spectroscopies. Batch and plug flow hydrogenation reactions of olefins and arenes were performed to highlight the catalytic activity of single-site and nanoparticulate metal centers.

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TECHNIQUES FOR SOLVING GLOBAL OPTIMUM OF BI-PARAMETRIC LINEAR PROGRAM WITH COMPLEMENTARITY CONSTRAINTS

A linear program with linear complementarity constraints (LPCC) is among the simplest mathematical programs with complementarity constraints. Yet the global solution of the LPCC remains difficult to find and/or verify. In this work we study a specific type of the LPCC which we term a bi-parametric LPCC. Such a bi-parametric LPCC arises from a typical training-and-validation parameter selection procedure, and the model to which the training-and-validation procedure applies has only two design parameters. We propose three algorithms for solving the global optimum of this problem. The first algorithm is a domain-partitioning branch-and-bound-like method that solves the relaxed linear subproblems, which generate valid lower bound, within each partitioned area. This algorithm terminates with global optimality when the gap between valid lower and upper bound is zero. The second algorithm is a rectangle-search method that searches the invariance regions (or pieces of LPCC, correspondingly) on the parameter plane. The algorithm is named 'rectangle'-search because we search along the boundaries of a rectangle and use the information obtained on the boundary to determine whether the interior points also belong to the same invariance regions discovered on the boundary. In contrast to the first algorithm, the solution obtained for each invariance region is a valid upper bound, and thus the algorithm terminates with global optimality when all invariance regions are realized. The third algorithm is a procedure to tighten the big-M value in an equivalent integer-program formulation of the bi-parametric LPCC. After obtaining the tightened big-M, the running time of solving the integer program by any commercial solver can be reduced. The solution to the integer program is equivalent to a global optimal solution to the bi-parametric LPCC in our scope of discussion.

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MASS-SELECTIVE DISCRIMINATION OF CHIRAL MOLECULES BY FEMTOSECOND COINCIDENCE IMAGING

Molecular chirality is a key property in chemistry and has intriguing consequences to living organisms. Optical detection of chirality is usually performed by circular dichroism of the probe light. However, this differential absorption is typically of the order of 0.01% to the total absorption cross-section. In 1976, Ritchie[1] reported that ionization with circular polarized light of randomly oriented gas-phase chiral molecules induces a forward-backward asymmetry of photoelectrons along the light propagation. Subsequently, using circular polarized synchrotron sources strong chiral asymmetries of up to 5-30% have been reported in one-photon ionization[2]. This chiral asymmetry in the photoelectron angular distribution is termed photo-electron circular dichroism (PECD). The high sensitivity of PECD makes angular-resolved photoionization of enantiomers very promising as a sensitive analytical technique to characterize chiral samples. Here we discuss our recent report[3,4] that a simple femtosecond table-top photo-electron photo-ion coincidence imaging set-up[5-7] can be used to detect mass-selected chiral molecules with remarkable sensitivity and high selectivity. This novel demonstration opens up the technique of PECD to small scale laser labs. Furthermore, the technique of multiphoton PECD enables the exploitation of excited intermediate states, two color pump-probe excitation and intermediate lab-frame alignment to enhance PECD.

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KIRKPATRICK-BAEZ MIRRORS TO FOCUS HARD X-RAYS IN 2-D ARE FABRICATED, TESTED, AND INSTALLED AT THE ADVANCED PHOTON SOURCE

We report on the design of the Kirkpatrick-Baez (K-B) mirrors mounting system, mirrors fabrication, and performance of the focus spot. The K-B mirror assembly is fully developed by the APS optics group and was designed for installation at 8-BM beamline. The two elliptical mirrors are arranged in sequential K-B optics. The mirrors are coated with Platinum (Pt) material on Si substrate. The vertical focusing mirror of 80 mm length with focal length of 255 mm and horizontal focusing mirror of 60 mm length with focal length of 155 mm. Magnetron sputtering deposition techniques was used to achieve the elliptical shape on the flat Si substrates. Metrology measurements showed that the figure errors for the 80 mm and 60 mm long mirror are 0.61 nm and 0.33 nm. A doubly focused $1.3(\text{vertical})\mu\text{m} \times 1.2(\text{horizontal})\mu\text{m}$ with monochromatic beam at 18keV was measured. The beamline layout, the techniques for characterizing the beam focal spot and performance of the mirrors are discussed.

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STOICHIOMETRIC AND CATALYTIC REACTIVITY OF TRIS(OXAZOLINYL)PHENYLBORATO ZINC AND MAGNESIUM COMPLEXES

Analogous to classic tris(pyrazolyl)borates, a new class of monoanionic tridentate ligand ToM [tris(4,4-dimethyl-2-oxazoliny)phenylborate] has been developed.¹ The corresponding monomeric complexes of Zinc and Magnesium (ToMMX; M = Zn, Mg) have been synthesized with special emphasis on alkyls and hydride as the terminal moieties (X).²⁻⁵ Subsequently, these are studied as catalysts for homogeneous organic transformations as well as stoichiometric activation of small molecules like O₂ and CO₂. ToMZnR (R= alkyl) forms monomeric zinc alkyl peroxides ToMZnOOR upon insertion of molecular O₂ at STP. ToMZnH catalyzes reductive hydrosilylation and hydroboration of carbonyls and dehydrogenative coupling of alcohols and hydrosilanes.^{3,6} ToMMgMe is an active pre-catalyst for reductive hydroboration of esters and carbonyls as well as Tishchenko dimerization of aldehydes.

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DENSITY FUNCTIONAL STUDY OF THE BPDE HYDROLYSIS REACTION

We computationally study three possible mechanisms for hydrolysis of benzo[a] pyrdene diol epoxide (BPDE) to its main tetrol: 1) spontaneous hydrolysis by a single water molecule 2) spontaneous hydrolysis where one water molecule acts as a proton donor in the rate limiting step 3) general acid catalysis, where cacodylic acid donates a proton in the rate limiting step. The computed activation energy of 3) matches well experimentally measured activation energies in neutral sodium cacodylate buffer. The acid catalyzed reaction most likely proceeds through a lower entropy hydrogen bonded acid-diol epoxide complex.

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SUB-WAVELENGTH METAMATERIALS: DESIGN, PHYSICS AND APPLICATIONS

Metamaterials, artificially structured nanomaterials, have enabled unprecedented phenomena such as invisibility cloaking and negative refraction. Especially, hyperbolic metamaterials also known as indefinite metamaterials have unique dispersion relation where the principal components of its permittivity tensors are not all with the same signs and magnitudes. Such extraordinary dispersion relation results in hyperbolic dispersion relations which lead to a number of interesting phenomena, such as super-resolution effect which transfers evanescent waves to propagating waves at its interface with normal materials and, the propagation of electromagnetic waves with very large wavevectors comparing they are evanescent waves and thus decay quickly in natural materials. In this abstract, I will discuss our efforts in achieving the unique optical property overcoming diffraction limit to achieve several extraordinary metamaterials and metadevices demonstration. First, I will present super-resolution imaging device called "hyperlens", which is the first experimental demonstration of near- to far-field imaging at visible light with resolution beyond the diffraction limit in two lateral dimensions. [1] Second, I will show another unique application of metamaterials for miniaturizing optical cavity, a key component to make lasers, into the nanoscale for the first time. It shows the cavity array which successfully captured light in 20nm dimension and show very high figure of merit experimentally. [2] Finally, if time allows, I will show the recent achievements of photo-induced switching of reconfigurable negative index metamaterial device and large scale negative index metasurface with anomalous spin-hall effect. [3, 4] I believe our efforts in sub-wavelength metamaterials having such extraordinary optical properties will lead to further advanced nanophotonics and nanooptics research.

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COMPUTATIONAL MODELING OF LITHIUM-OXIDE NANOSYSTEMS FOR LI-AIR BATTERY APPLICATIONS

We investigate nanocrystalline lithium oxide compounds, including Li₂O and Li₂O₂, by molecular dynamics simulations in order to gain insight into crystal growth processes relevant to lithium-air batteries which are difficult to observe directly by experiment. Due to its cubic structure, Li₂O is used as a simple model system to systematically develop MD simulations of the structure and properties of surfaces, individual nanoparticles and fully dense nanocrystalline microstructures. Lithium peroxides, Li₂O₂, are more complex materials which require a more sophisticated model to describe nucleation and crystal growth. We develop a flexible many-body, variable charge interionic potential to model crystalline lithium-oxide materials in any stoichiometric ratio.

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LARGE TUNABLE INDUCTANCE OF THE DECORATED JOSEPHSON CHAIN

We discuss the new design of a tunable superconductive inductance made from the decorated frustrated Josephson junction chains frustrated by magnetic field. We show that for the optimal choice of parameters the inductance of this chain varies in a very wide range as a function of the magnetic field. The resulting plasma frequency may exceed the value of quantum resistance, that characterizes superinductance. The important distinction of this design from the chain of dc-SQUIDS loops is the absence of phase slips at all magnetic fields. We present the results of the extensive numerical simulations that confirm these expectations.

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MICROBIAL NITROGEN CYCLING POTENTIAL IS DRIVEN TOWARDS AMMONIUM PRODUCTION DURING POLYAROMATIC HYDROCARBON POLLUTION IN MARINE SEDIMENTS

Petroleum hydrocarbon spills considerably alter the composition and functional dynamics of marine microbial communities. Ultimately, microorganisms that can respond to the complex hydrocarbon mixture are unlikely to significantly proliferate in the absence of the spill, and hence probably grow from small natural seed populations. Light hydrocarbons, such as alkanes, are oxidized aerobically and quickly assimilated into microbial biomass, on a time scale of days to weeks, while highly recalcitrant, polyaromatic petroleum residues undergo very slow degradation and, once buried in anaerobic sediment, remain detectable for many decades. The process of hydrocarbon degradation is heterotrophic, causing a localized reduction in oxygen potential in marine sediments. Here we hypothesize that increasing exposure to elevated hydrocarbon concentrations will positively correlate with direct oxidation of ammonium to dinitrogen through the Anaerobic Ammonium Oxidation (ANAMOX) pathway, and a shift towards direct reduction from nitrite to ammonium through dissimilatory nitrate reduction to ammonium (DNRA), due to localized heterotrophic respiration leading to depletion of oxygen. This hypothesis was tested by comparing the relative abundance of genes associated with nitrogen cycling in 6 metagenomes sequenced from uncontaminated sediments, 8 from sediments contaminated by polyaromatic hydrocarbons from the Deepwater Horizon oil spill, and 5 from natural oil seeps that occur in the Santa Barbara Channel. Following annotation of gene function from sequenced fragments in each metagenome, the annotated enzyme abundances were quantile normalized and log transformed. We used predicted relative metabolic turnover (PRMT) to explore relative changes in metabolic activity as a function of the microbial community, and used the summed directional PRMT scores to determine the 'net' flow of nitrogen-associated metabolism. A shift in the metabolic flow of nitrogen to the ANAMOX pathway was observed in the contaminated samples (both oil spill and natural oil seep), and the magnitude of this change was positively correlated to the hydrocarbon concentration and inversely correlated with oxygen concentration in these sediments. The number of bacterial taxa associated with ANAMOX physiology was also shown to increase along the gradient of hydrocarbon pollution. Marine sediments are very important sites for microbially mediated nitrogen transformation, providing a link between organic matter degradation and nutrient regeneration, essentially supporting primary productivity in the oceans. Exploring factors that significantly influence this process are vital for providing relevant data to propagate system scale models of how basin processes such as nitrogen cycling and primary productivity in the Gulf of Mexico can influence regional and global climate.

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ENGINEERING POROUS ORGANIC POLYMER CATALYSTS

Porous organic polymers (POPs) are highly porous cross-linked networks that are built from multi-topic organic linkers. Depending on the choice of organic linker used, POP topology and functionality can be readily modified through pre- or post-synthesis methods to enhance their host-guest interactions for gas storage/separation and catalytic applications. Recently, POPs have demonstrated excellent chemical (e.g., acid and base) and environmental (i.e., temperature and pressure) stabilities, therefore making them attractive supports for heterogeneous catalysis. This presentation focuses on the development of POP catalysts with well-defined active sites. Synthesis and characterization, catalytic testing, and substrate-catalytic site interactions with these POP materials will be discussed.

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UNDER-HOOD THERMAL ANALYSIS FOR OPTIMIZATION OF HEAVY VEHICLES

In automotive industry, the efficient under-hood thermal management of an engine cooling system and its surrounding components are highly desirable to make fuel efficient vehicles. To optimize the under-hood performance, several numerical experiments are carried using Computational Fluid Dynamics (CFD) tool to improve the new/existing designs. In this work, thermal analysis is performed for under-hood design of heavy-vehicle using STAR-CCM+. The external airflow cooling is performed by varying geometry configurations and operating conditions of fan and heat exchangers including modified side edges, fan blade angles and flow resistances across the Charge Air Cooler (CAC) and radiator. The observed temperatures in CAC and radiator using the modified side edges drops to value of 2 oC as compared to base case. This is mainly due to the high cross sectional flow surface area in the modified design. On the other hand, the significant reduction of the temperature predicted with fan blade angles. The highest reduced temperature observed at 45o fan blade angle. This is mainly due to the high pressure drop that leads to high flow rates. Moreover, with lowering the flow resistance across the CAC and radiator also reduces the temperature as compared to the base case. Finally, the placing of the components, i.e. CAC, radiator, shroud, fan and engine also affects the flow patterns and the temperature profiles. Moreover, an additional component like flaps helps to avoid hot spots in the heat exchanges. Gap sensitivity analysis of CAC and radiator shows significant effects on the flow and temperature profiles.

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BUILDING AFFINITY MATURATION INTO THE PHAGE DISPLAY PIPELINE OF DESIGNER AFFINITY REAGENTS

Protein engineering is an effective means by which to generate affinity reagents capable of binding human biomarkers with superior affinity and specificity. Such reagents would be extremely useful in research, diagnostic and therapeutic applications. The development of a high-throughput pipeline for the production of these affinity reagents would allow for them to be prepared quickly, in a tailor-made fashion, and readily available to the community on demand. Our laboratory is currently developing an efficient method for generating high affinity reagents, based on the fibronectin type III (FN3) monobody scaffold, via M13 bacteriophage display. To enhance the output of the affinity selections, we have incorporated affinity maturation through mutagenic PCR and loop shuffling into the selection process itself, resulting in an improvement in affinities for a large number of binders. To demonstrate the utility of this new method, we generated affinity reagents with low nanomolar Kd values for three human targets: ubiquitin-conjugating enzyme E2 R1 (CDC34), mitogen-activated protein kinase kinase 5 (MAP2K5) and ubiquitin carboxy-terminal hydrolase 11 (USP11). This work was supported by grant 1 U54 DK093444-01 from the National Institutes of Health (NIH).

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QUANTITATIVE INSIGHTS INTO NEXT GENERATION BATTERIES FROM HARD X-RAY

The advancement of mobile electronic devices has driven the demand for more efficient electrical energy storage systems. Next-generation batteries, based on conversion reactions, promise higher capacities than conventional intercalation-based systems. During the conversion reaction an oxidized transition metal compound is fully reduced to the zero valent metallic state. As a consequence, the electrode restructures completely. The metal and one or more other phases are produced. These multiple phases must recombine upon charging. The complex nature of the reaction and recombination underlies an often incomplete reversibility of each discharge and charge cycle and hence, a progressive capacity loss. However, it is difficult to predict ab initio which electrode candidates will perform best. Accordingly, understanding conversion reaction mechanisms is critical to the development of batteries. Iron oxides, fluorides and oxyfluorides provide an interesting series in which to study conversion reactions. While the bulk materials suffer from poor electronic and ionic conductivity, smaller particles – on the nanoscale – show improved electrochemical performance. Moreover, the nanostructure of the starting electrode and reaction products present a significant characterizations challenge. Pair Distribution Function (PDF) analysis and Small Angle X-ray Scattering (SAXS) are ideally suited to probing nanostructured materials. PDF analysis can provide comprehensive insights into

the electrochemical reaction mechanism and the changes in local and intermediate-range atomic structure. SAXS provides insight into the nanoparticle size, shape, size distribution and packing. Here we use a custom-designed electrochemical cell for operando X-ray studies of high performance iron oxide, fluoride and oxyfluoride electrodes. We explore the nanoparticle formation and ripening in series of Fe-based conversion materials.

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HARD X-RAY ZONE PLATE DEVELOPMENT AND APPLICATION AT ADVANCED PHOTON SOURCE

Zone plates are diffractive focusing optics, similar to circular diffraction gratings but with changing period as a function of radius. The optics offer fine resolution, controllable focal length, and 2-D focusing in a thin optic that is simple to align (1). Though the focusing efficiency is limited and this limitation is made worse due to the zone plates for fine resolution being far from ideal in efficiency. Hard X-ray zone plates are used as the objective optic in the new transmission X-ray microscope (TXM) at Sector 32-ID-C of the Advanced Photon Source (APS). The TXM as well as other beamlines at APS are driving zone plate development for finer resolution with peak efficiency at high X-ray energy. Hard X-ray zone plates with 20-nm-resolution and peak efficiency will require outer zones with aspect ratio greater than 100. The large aspect ratio poses the greatest challenge to fabrication of efficient zone plates. We will present the latest work in zone plate development at APS, as well as some results of 20-nm-outer zone width zone plates at the new TXM.

Zone plate developments that will be presented have concentrated on improving previously established processes such as zone doubling (2) and zone plate stacking (3). Work with zone plate stacking was done for an intermediate zone plate stacking technique (4). Aligning optics in the TXM require several steps to set up the tool to image samples. With all optics aligned in the TXM, images were taken of Siemens stars with 50 nm and 100 nm inner spoke. The Siemens star images were used as a test of resolution, and efficiency measurements were also done. The data will be used to characterize fabricated zone plates, and at the same time demonstrates the capabilities of the TXM.

There were several sets of zone plates fabricated using different techniques depending on dimension required. A zone doubling technique was used to fabricate 20-nm-outer zone width zone plates for the TXM. There are two primary steps in the zone doubling fabrication method, and the zone plate structure after lithography is shown in Figure 1. The line quality in the pattern is very consistent, which was a result of the work done in developing the lithography recipe. Fully fabricated zone doubled zone plates and intermediate stacked zone plates will be presented as well. The new TXM at Sector 32-ID-C was designed to use zone plates for 20 nm resolution images. A 50 nm inner spoke Siemens star was imaged at 8 keV X-ray energy and shown in Figure 2. Fabrication defects in the star can be clearly seen, which suggests better than 50 nm resolution. Information on the work done with the TXM will be presented as well.

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ROLE OF LiNO_3 AS A SHUTTLE INHIBITOR IN LITHIUM SULFUR BATTERIES

LiNO_3 was found to be an effective shuttle inhibitor in Li-S batteries. To better understand how it functions, we conducted an experiment to determine 1) whether LiNO_3 worked as a catalyst or whether it was consumed during the cycling of the cell, and 2) whether the shuttle-inhibiting function was provided by the formation of a protective layer on the lithium metal, or by the continuous reaction between LiNO_3 and lithium metal and/or reduced lithium polysulfides. We prepared lithium polysulfide electrolytes having increasing concentrations of LiNO_3 . The polysulfides in the electrolyte functioned as lithium salts and increased the shuttle reactions, which provided a good condition for studying the effect of LiNO_3 additive. We found that LiNO_3 was consumed continuously during cycling, and the coulombic efficiency of the cell decreased as the amount of LiNO_3 initially present in the electrolyte decreased. We next conducted an experiment to determine whether the shuttle-inhibiting function was provided by the formation of a protective layer on the lithium metal, or by the continuous reaction between LiNO_3 and lithium metal and/or reduced lithium polysulfides. A cell containing a sulfur electrode and a fresh lithium metal was first tested using an electrolyte of 0.5M LiNO_3 in DME. The cell was charged and discharged for 16 cycles and had an efficiency of almost 100% for all the cycles (Fig. 1a and b). After testing, we opened the cell, removed the lithium metal, and recycled it in a cell using a new sulfur electrode with the conventional electrolyte, which was 1M LiTFSI in DME/DOL. As shown in Fig. 1c and d, this new cell had shuttle reactions very much the same as other lithium-sulfur cells using the LiTFSI-based electrolyte without any LiNO_3 . The recycled lithium metal with protective layer did not suppress the shuttle reactions in the new cell. We concluded that the shuttle-inhibiting mechanism of the LiNO_3 additive involves continuous reactions with other species rather than the formation of a passivation layer on the lithium anode.

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Argonne National Laboratory, Chemical Sciences and Engineering

CROSS-LINKABLE URETHANE ACRYLATE OLIGOMERS AS BINDERS FOR LITHIUM-ION BATTERY

The demand for next-generation lithium-ion batteries requires not only the discovery of new electrode materials, but also the concurrent development of other active and inactive components in a lithium-ion battery. To this end, a variety of polymers that are tailored to meet specific needs have been investigated as binders for different electrode materials. However, polymer binders with desired functionalization require much synthetic effort before they can be evaluated in the cell. We developed a method to fabricate electrodes using cross-linkable, low molecular weight oligomers as binder precursors. Electrode laminates of $\text{LiNi}_{1/3}\text{Mn}_{1/3}\text{Co}_{1/3}\text{O}_2$ (NMC) cathode cured with a urethane acrylate oligomer-based binder were prepared via a free-radical initiated polymerization process. The physical properties of the cured electrodes were found to depend on the composition of the binder. NMC electrode cured with the optimized binder formulation was evaluated electrochemically in NMC/Li and NMC/MCMB cells, which exhibited excellent cycling and C-rate performance. The advantage of this approach is that it benefits from a broad selection of functional, reactive oligomers, which allows for the easy tuning of the binder structure to afford the desired physical and electrochemical properties of the electrode.

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INCORPORATION OF HALOGEN OXIDANTS INTO PROPANIOIC ANHYDRIDES DERIVED FROM NICKELALACTONES

Nickelacyclic carboxylates, derived from oxidative coupling of CO_2 and ethylene, offer an intriguing system to study catalytic reactions that utilize CO_2 as a C1 building block. Nickelalactones can undergo three general stoichiometric reactions: 1) insertion of CO to generate the corresponding succinic anhydrides; 2) C-C coupling with halogenated alkanes; 3) Formation of dicarboxylic acids by insertion of C_2H_4 , CO_2 , and CO in the presence of BeCl_2 and pyridine. The fate of the resulting nickel complexes were not investigated due to the aqueous acidic work up used to isolate the organic products. We became interested in these complexes to develop novel catalytic reactions involving CO_2 and olefins.

All experiments were performed under a nitrogen atmosphere using standard Schlenk and glovebox techniques. NMR Spectra were recorded on Bruker DMX-500 spectrometer in Teflon-valved tubes at ambient temperature unless otherwise indicated. Electrospray mass spectra (ESI-MS) were recorded on freshly prepared samples using an Agilent 1100 LC-MSD spectrometer.

Initial investigations reacting $(\text{dppe})\text{Ni}(\text{C}_2\text{H}_4\text{CO}_2)$ (dppe = 1,2-bis(diphenylphosphino)ethane) with excess dihalogen revealed the formation of 3-X-propionic anhydrides ($\text{X} = \text{Cl}, \text{Br}, \text{I}$) with concomitant formation of $(\text{dppe})\text{NiX}_2$ and $[(\text{dppeO}_2)_3\text{Ni}][\text{NiX}_4]$.

It was hypothesized that a key intermediate in the formation of the anhydride is a $(\text{dppe})\text{NiX}(\text{O}_2\text{CR})$ species ($\text{X} = \text{Cl}, \text{Br}, \text{I}$). Attempts to prepare such complexes using $\text{Ti}(\text{O}_2\text{CtBu})$ and $(\text{dppe})\text{NiBr}_2$ led to the formation of $(\text{dppe})\text{NiBr}_2$, $[(\text{dppe})_2\text{Ni}][\text{Ni}(\text{O}_2\text{CtBu})_4]$, and $(\text{dppe})\text{Ni}(\text{O}_2\text{CtBu})_2$ (Scheme 2). Conversely, this mixture of complexes could be generated using equal amounts of $(\text{dppe})\text{NiBr}_2$ and $(\text{dppe})\text{Ni}(\text{O}_2\text{CtBu})_2$. These results taken together, suggest that rapid ligand redistribution reaction occurs in solution. Oxidation of this mixture of compounds resulted in the formation of $(\text{dppe})\text{NiBr}_2$, pivalic anhydride and $[(\text{dppeO}_2)_3\text{Ni}][\text{NiBr}_4]$.

Additionally, mixing the known $(\text{dppe})\text{NiBr}_3$ and $\text{Na}(\text{O}_2\text{CtBu})$ led to formation of NaBr and the same products (Scheme 2). These results suggest that oxidation must occur before extrusion of the final products.

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PERFLUOROALKYL-SUBSTITUTED ETHYLENE CARBONATES: NOVEL ELECTROLYTE ADDITIVES FOR HIGH-CAPACITY LITHIUM ION BATTERIES

High-capacity lithium- and manganese-rich metal oxides are gaining increased attention because of their ability to deliver high rechargeable capacities; when cycled between 2.0 and 4.7 V vs. Li, a rechargeable capacity of 270 mAh-g⁻¹ can be routinely obtained.[1] Hence lithium-ion cells containing the Li_2MnO_3 -stabilized LiMO_2 ($\text{M} = \text{Mn}, \text{Ni}, \text{Co}$) positive electrodes, graphite negative electrodes and EC:EMC (3:7 by wt.) + 1.2 M LiPF_6 -based electrolyte (henceforth referred as Gen2 electrolyte) can be designed to meet the target cell specific capacity of ~250 Wh-kg⁻¹ for transportation applications.[2, 3] However, the target battery cycle life of up to 1000 charge-discharge cycles at 80% depth of discharge (DOD) can only be achieved through new electrolyte formulations because these cells show significant performance degradation on extended cycling.[4] Extensive diagnostic studies indicate that cell impedance rise mainly arises at the positive electrode, and cell capacity fade mainly results from lithium trapping in the solid electrolyte interphase (SEI) at the negative electrode.[4-6] During electrochemical aging, both electrodes undergo a cycle of surface film formation, decomposition, dissolution, and redeposition; this process results in continuous consumption of lithium ions, thereby reducing cell capacity and often increasing cell impedance.

Electrolyte additives are known to be an effective and economic approach to improving the stability of electrode surface films.[7] In the past two decades, many organic and inorganic compounds have been identified as effective electrolyte additives: examples include vinylene carbonate (VC), ethylene sulfite (ES), vinyl ethylene carbonate (VEC), and fluoroethylene carbonate (FEC). In recent years, with the emergence of many high-voltage cathode materials, the anodic stability of common electrolytes

is recognized as the main bottleneck limiting the calendar- and cycle- life of high-energy lithium-ion cells.[8] Therefore, more attention has been devoted to improving stability of the cathode–electrolyte interface. As part of DOE's Advanced Battery Research (ABR) program, we have been examining ways to mitigate performance degradation of cells containing $\text{Li}_{1.2}\text{Ni}_{0.15}\text{Mn}_{0.55}\text{Co}_{0.1}\text{O}$ -based positive electrodes (LMR-NMC) that are cycled at voltages beyond 4.5 V versus Li. Initial studies indicate that common electrolyte additives such as VC, VEC, and FEC are not effective at enhancing long-term cycling performance of these cells, i.e. stable electrode passivation could not be achieved with traditional SEI-forming additives. This observation underscores the need for new electrolyte additives that effectively form stable electrode passivation films in high-energy and high-voltage lithium-ion cells.

Polyfluoroalkyl (PFA) compounds are well known for their high chemical stabilities, and exhibit both hydrophobic and lipophobic behaviors. Upon dispersing in organic solvents, solvophobic PFAs tend to aggregate and form micelles in solution.[9] In light of these facts, we envision that PFA compounds can serve as a new type of electrolyte additive. In our design, the PFA additive has two components: (i) a reactive head-group for attachment onto electrode surfaces via either reductive or oxidative decomposition, so that it becomes an integral part of the surface layer; (ii) a polyfluoroalkyl chain that self-assembles on the electrode surface into a solvophobic passivating layer that reduces both surface degradation and electrolyte decomposition.

To explore this novel idea, we synthesized a series of PFA-substituted ethylene carbonates and studied them as electrolyte additives in our high-voltage lithium-ion cells. The battery cycling performance was characterized using a combination of galvanostatic cycling and electrochemical impedance spectroscopy (EIS) techniques, and supplemented by X-ray photoelectron spectroscopy (XPS), scanning electron microscope (SEM) and Raman spectroscopy data. Within this series of compounds studied, we determined that perfluorooctyl-substituted ethylene carbonate (PFO-EC) most significantly improved the long-term cycling performance of our cells.

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Argonne National Laboratory Postdoctoral Research and Career Symposium

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