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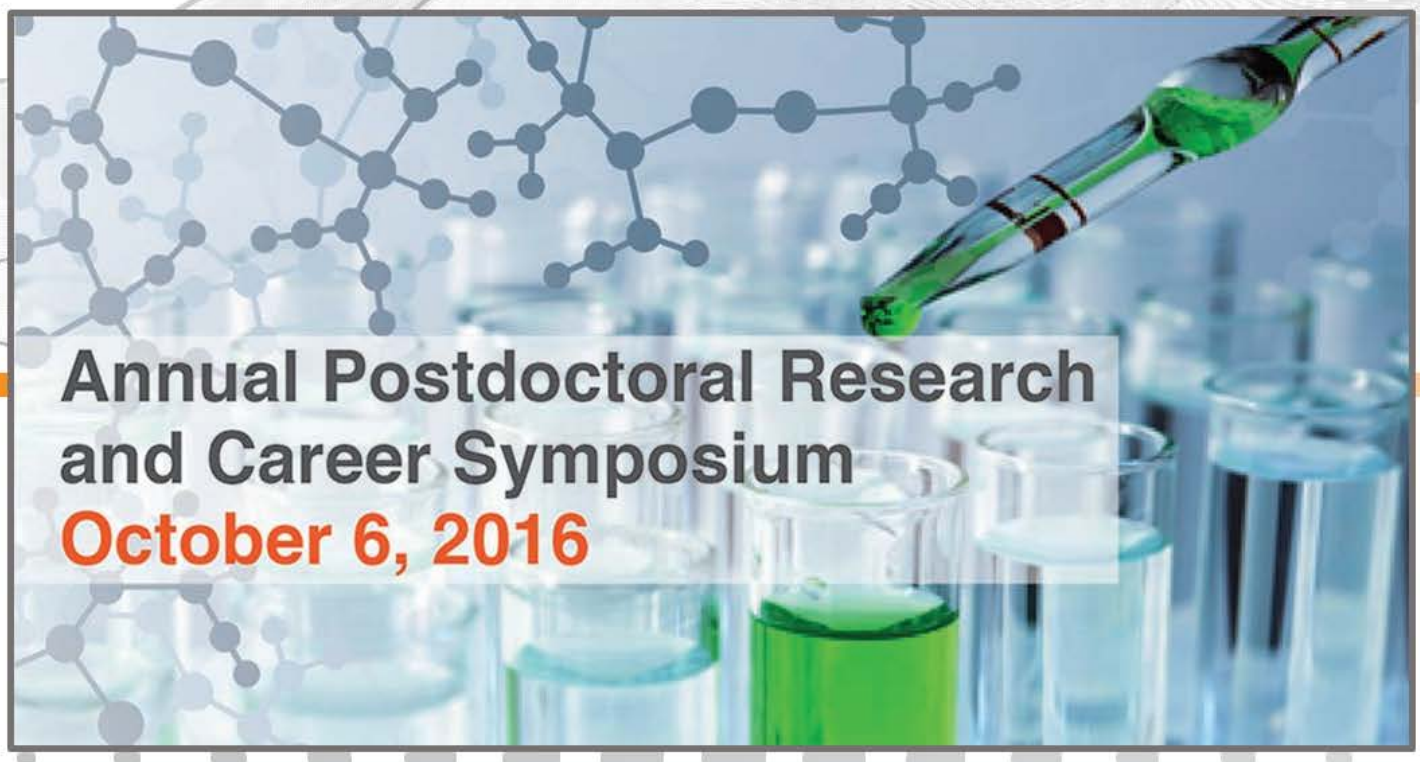

Annual Postdoctoral Research and Career Symposium

October 6, 2016

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Argonne National Laboratory Postdoctoral Research and Career Symposium

October 6, 2016

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2016 Postdoctoral Research and Career Symposium
October 6, 2016

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2016 Postdoctoral Research and Career Symposium
October 6, 2016

Agenda

8:30 AM — Continental Breakfast and Registration (TCS Conference Center)

MORNING SESSION

9:00 AM — Welcome Remarks from Alfred Sattelberger, Deputy Director for Programs, Argonne National Laboratory

9:15 AM — Keynote Address by Christopher DellaCorte, NASA, Glenn Research Center
"NiTi Alloys for Tribological Applications: The Effects of Serendipity on R&D"

10:15 AM — Academic Panel Discussion: "Navigating Academic Careers"

Prof. Yip-Wah Chung, Northwestern University
Dr. Connie Lee, University of Chicago
Prof. Walter Henne, Governors State University
Prof. Darya Aleinikava, Benedictine University

10:55 AM — Break

11:10 AM — Non-Academic Panel Discussion: "Opportunities in Non-Academic Careers"

Dr. Hendrik Hamann, IBM T.J. Watson Research Center
Dr. Anton Spirkin, ExxonMobil Upstream Research Company
Dr. Carlton Reeves, ARPA-E, Department of Energy
Dr. Elena Shevchenko, CNM, Argonne National Laboratory
Dr. Suresh Sunderrajan, TDC, Argonne National Laboratory

11:50 AM — Poster and Booth Set-Up

NETWORKING LUNCH

12:10 PM — Networking Lunch Kickoff by Justin H. S. Breaux, Communications Specialist, Argonne National Laboratory

12:30 PM — Networking Lunch (company exhibitors and representatives from diverse career paths will have a chance to talk with postdocs in small groups)

AFTERNOON SESSION

2:00 PM — Poster Session and Career Booth Assembly

2:15 PM — Poster Session A and Company Exhibits

3:15 PM — Poster Session B and Company Exhibits

4:15 PM — Networking Reception and Company Booth Time

5:30 PM — Presentation of Poster Awards

6:00 PM — Closing Remarks

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2016 Postdoctoral Research and Career Symposium
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2016 Keynote Address

NiTi Alloys for Tribological Applications: The Effects of Serendipity on R&D

Christopher DellaCorte. , NASA, Glenn Research Center

Novel superelastic materials based upon Nickel-Titanium (NiTi) alloys are an emerging solution that almost escaped recognition. Though steel is the dominant material of choice for mechanical components (bearings, gears, transmissions) it has intrinsic limitations related to corrosion and plastic deformation. In 2004, at the request of a small manufacturing firm, Nitinol 60 was assessed as an alternative to bearing steel. It was shown to be hard and impervious to aqueous corrosion but its tribological properties were largely unknown. Conventional wisdom in the field of tribology suggests that alloys rich in titanium are poor candidate bearing materials but NiTi, an intermetallic, demonstrates that such thinking can be and often is, wrong. Though early stage tests reveal acceptable friction and wear behavior, extensive materials engineering and processing development was needed to produce the precision microstructures needed for long-life bearings and gears. In the course of exploring this new material system other game-changing and unexpected properties, such as superelastic resilience, were observed. Today, the aerospace community is exploiting the unique characteristics of the NiTi alloy system to solve problems on earth, underwater and in space. A fortunate decision to consider a single industrial request turned out to be the key to an entirely new technologically.

Dr. Christopher DellaCorte, Senior Technologist: Tribology and Rotating Machinery, Materials and Structures Division, Research & Engineering Directorate, NASA, Glenn Research Center.

Dr. DellaCorte applies mechanism and tribology expertise to lead complex root cause failure investigations with a successful, proven track record. Examples include deciphering the International Space Station (ISS) Solar Alpha Rotary Joint (SARJ) failure mechanism, guiding the rotordynamic analyses of the Mars Science Laboratory Surface Analysis on Mars vacuum pump bearing failures. He leads a research team developing Nickel-Titanium based corrosion immune and shockproof bearings and gears to help avoid future tribology problems in aerospace systems.

Dr. DellaCorte began his NASA career in 1985 as a graduate student in the Surface Science Branch. In 1987, shortly after earning a Master of Science degree in mechanical and aerospace engineering from Case Western Reserve University (CWRU) he was hired as a permanent employee to work on tribology (friction and wear) problems for extreme environments. Early career highlights include developing an understanding of the friction and wear behavior of emerging engineered ceramics that were then candidates for advanced heat engines and aerospace vehicle airframes and structures. Much of this research became the basis for his Ph.D. dissertation (CWRU, 1989).

Dr. DellaCorte's technical accomplishments and contributions, over his career, have earned him prestigious recognitions including; the NESC Engineering Excellence Award, NASA Space Flight Awareness Award, NASA Qasar Award for the ISS SARJ Failure Analysis, NASA Silver Snoopy Award, the NASA Exceptional Service Medal, two R&D 100 Awards, and the Federal Laboratory Consortium Award for Commercialization. In addition to eight awarded patents on tribology technologies, Dr. DellaCorte has published well over 100 peer-reviewed papers and journal articles in more than 12 professional journals and numerous proceedings and has hundreds of citations.

Dr. DellaCorte's work is recognized nationally and internationally and he is an active professional society leader attaining Fellow rank in the American Society of mechanical Engineers (ASME) and the Society of Tribologists and Lubrication Engineers (STLE). He was the founding editor of STLE's monthly publication Tribology and Lubrication Technology. He is now the Editor-In-Chief of the peer-reviewed journal Tribology Transactions. He previously served two terms on STLE's board of directors.

Welcome Remarks Speaker

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

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

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

Academic Careers Panelists

Prof. Yip-Wah Chung, Department of Materials Science and Engineering and Mechanical Engineering, and Co-Director, Institute for Sustainability and Energy, Northwestern University

Yip-Wah Chung obtained his BS (physics and mathematics) and MPhil (physics) degrees from the University of Hong Kong, and PhD (physics) from the University of California at Berkeley. He then joined the Department of Materials Science and Engineering at Northwestern University in 1977. He served as Director of the Center for Engineering Tribology at Northwestern from 1987 to 1992, as Department Chair from 1992 to 1998, and as program officer in surface engineering and materials design at the U.S. National Science Foundation from 2003 to 2005. He has served many years in the Research Grants Council and University Grants Committee of Hong Kong. He has published over 200 papers in surface science, thin films, tribology, and alloy design, two textbooks (Practical Guide to Surface Science and Spectroscopy, Introduction to Materials Science and Engineering), one monograph (Micro- and Nanoscale Phenomena in Tribology) and was the co-editor of a six-volume Encyclopedia of Tribology. Current research studies include hard coatings, high-performance steels, and advanced lubricants for improved vehicle efficiency. He was named Fellow, ASM International; Fellow, AVS; and Fellow, Society of Tribologists and Lubrication Engineers. His other awards include Teacher of the Year in Materials Science, Innovative Research Award and Best Paper Awards from the ASME Tribology Division, Technical Achievement Award from the National Storage Industry Consortium, Bronze Bauhinia Star Medal from the Hong Kong SAR Government, Advisory Professor from Fudan University, and Visiting Fellow from Japan Society for Promotion of Science. He is also a commercial pilot and an advanced/instrument ground instructor.

Dr. Connie M. Lee, Associate Dean for Basic Science, Biological Sciences Division, The University of Chicago

Connie is currently the Associate Dean for Basic Science in the Biological Sciences Division at the University of Chicago, where she helps oversee the basic science research and graduate education mission in the Biological Sciences Division. She is a cell biologist by training, and received her PhD in the Molecular and Cellular Biology Program from the University of Wisconsin-Madison. After a postdoctoral fellowship at the Ludwig Maximilian University of Munich working on protein import into mitochondria, she transitioned into scientific editing and publishing. Connie worked for 11 years as a scientific editor for three different journals, including FEBS Letters, EMBO Journal, and most recently as Deputy Editor of Cell. As an editor, Connie was responsible for evaluating scientific papers, managing the peer-review process, recruiting high quality content to the journal, and working with authors to convey the importance of their work. In 2011, Connie left the editorial field and went back to an academic setting, taking the Associate Director & Scientific Coordinator role at the newly NIH-funded Center for Systems & Synthetic Biology at University of California San Francisco (UCSF). She was responsible for overseeing day-to-day operations of the Center, including strategic and financial planning, infrastructure and administrative organization, progress reporting, internal scientific meetings and external symposia, educational and outreach activities, and establishing a new Systems Biology Fellows program for independent, early-stage investigators. Connie has organized several international scientific workshops and conferences while at Cell and during her time at UCSF. In addition to her duties as Associate Dean, she continues to develop her interests in science policy and advocacy, the communication of science, and in career opportunities for scientists. She remains active in the scientific community by serving on the Public Policy Committee for the American Society for Cell Biology, where she has been Chair since 2014.

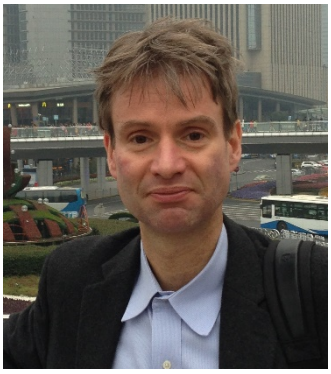
Prof. Darya Aleinikava, Assistant Professor, Physics and Engineering, Benedictine University

Darya Aleinikava completed her undergraduate studies at Belarusian State University, Belarus, and received her Master's and Doctoral Degrees in Physics from the City University of New York, New York. Her graduate thesis was on the topic of quantum dislocations in solid He4. After obtaining her PhD, Darya spent a year and an half as a Postdoctoral Appointee at Argonne National Lab, working together with Dr. Julius Jellinek in the CSE division. Darya's postdoctoral studies were in the field of fundamental developments in theory of nanoscale materials. She joined the Physics and Engineering department at Benedictine University, Lisle, three years ago, where she is now Assistant Professor of Physics. Darya's last publication was featured as an Argonne press release in August, 2016.

Prof. Walter Henne, Associate Professor of Chemistry, Governors State University

Walter Henne is Associate Professor of Chemistry at Governors State University. Walter received his Ph.D. in Chemistry from Purdue University with a special focus in Bio-Analytical Chemistry and Chemical Biology. He performed research at Purdue as part of the Philip S. Low Research Laboratory. His current research centers on the design of medical diagnostic assays, devices and targeted chemotherapeutics. He is the author of more than 20 peer-reviewed research papers and patents. Walter's experience spans the government, academic and industrial spheres. In addition to working as an analytical chemist and pilot plant liaison at a large chemical production facility he also worked as a supervisor in a medical facility dealing with patient care.

Non-Academic Careers Panelists



Dr. Hendrik F. Hamann, Research Manager for Physical Analytics, IBM T.J. Watson Research Center

Dr. Hendrik F. Hamann is a Distinguished Research Staff Member and Senior Research Manager in the Physical Sciences Department at the IBM T.J. Watson Research Center, in Yorktown Heights, NY. He received his PhD from the University of Goettingen in Germany. In 1995 he joined JILA (joint institute between the University of Colorado and NIST) as a Research Associate in Boulder, Colorado. During his tenure at JILA, he developed novel, near-field optical microscopes to study single molecules at high spatial resolution. Since 2001 he has led the Physical Analytics program in IBM Research. Between 2005 and 2009 he worked on energy management from the device level all the way to large scale computing systems. His current research interests include the combination of physical model, machine-learning and big data technologies, internet of things, sensor networks, sensor-based physical modeling, and system physics with applications in renewable energy, precision agriculture, and energy management. He has authored and co-authored more than 80 peer-reviewed scientific papers, holds over 90 patents, and has over 70 pending patent applications. Dr. Hamann is an IBM Master Inventor, a member of the IBM Academy of Technology, and has served on governmental committees such as the National Academy of Sciences, the National Science Foundation and as an industrial advisor to universities. He is a member of the American Physical Society (APS), Optical Society of America (OSA), The Institute of Electrical and Electronics Engineers (IEEE) and the NY Academy of Sciences.

Dr. Carlton Reeves, Technology-to-Market Advisor, Advanced Research Projects Agency-Energy, U.S. Department of Energy

Dr. Carlton Reeves is a Technology-to-Market Advisor at the Advanced Research Projects Agency – Energy (ARPA-E). He is responsible for leading the path to market approach for several programs including the Traveler Response Architecture using Novel Signaling for Network Efficiency in Transportation (TRANSNET), NEXT-Generation Energy Technologies for Connected and Automated on-Road-vehicles (NEXTCAR), and Network Optimized Distributed Energy Systems (NODES). He also assists a wide variety of other ARPA-E Tech-to-Market efforts, preparing breakthrough energy technologies for transition from lab to market.

Prior to joining ARPA-E, Reeves worked with President Obama's Council of Advisors on Science and Technology (PCAST) at the White House Office of Science and Technology Policy (OSTP). Preceding his time at OSTP, Reeves was the Entrepreneur-in-Residence at the University of Wisconsin Milwaukee Research Foundation where he worked closely with student and faculty entrepreneurs by helping them bring their novel ideas and research to market. Reeves provided the knowledge and assistance needed to evaluate commercial opportunities, define business models, develop business plans, and identify resources to advance early stage enterprises.

Reeves has launched several of his own businesses and is a published author. He was also named a University Innovation Fellow, a joint venture between Stanford University's National Center for Engineering Pathways to Innovation and VentureWell. Reeves holds a Ph.D. from the University of Wisconsin Milwaukee and B.S. and M.S. in Mechanical Engineering from Carnegie Mellon University.

Dr. Anton Spirkin, High Performance Computational Projects, Seismic Computation and Inversion, ExxonMobil Upstream Research Company
B.S. & M.S. Moscow Institute of Physics and Technology, Applied Physics and Mathematics
Ph.D. Worcester Polytechnic Institute, Mechanical Engineering
Research background includes rarefied gas dynamics, combustion and computational plasma physics.
Since 2007: Research Associate, ExxonMobil Upstream Research Company
Currently a member of the Computational Sciences Function – High Performance Computational Projects – Seismic Computation and Inversion team.
Developed novel numerical algorithms in the areas of seismic imaging (e.g. Full Waveform Inversion), reservoir modeling, data mining and pattern recognition.

Dr. Elena Shevchenko, Scientist, Center for Nanoscale Materials, Argonne National Laboratory.

Elena Shevchenko is a scientist at the Center for Nanoscale Materials at Argonne National Laboratory. She received her first degree in chemistry at the Belorussian State University and her PhD from the University of Hamburg in 2003 with Horst Weller. From 2003 to 2005 she was a joint postdoctoral fellow at Columbia University and IBM T.J. Watson Research Center. In 2005, she moved to the Molecular Foundry at Lawrence Berkeley National Laboratory as a staff scientist. Her research interests include the synthesis of nanoscale materials with controllable size and shape, design of multifunctional materials through self-assembly of nanoparticles, and study of the collective properties of such materials.

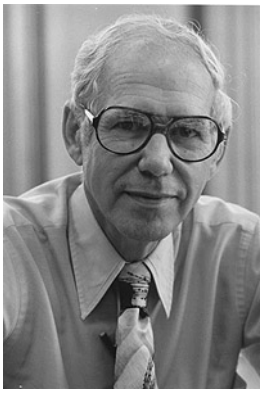
Dr. Suresh Sunderrajan, Division Director, Technology Development and Commercialization, Argonne National Laboratory
Suresh Sunderrajan is the Division Director of the Technology Development and Commercialization (TDC) Division and Chief Commercialization Officer at Argonne National Laboratory.
Suresh came to Argonne from United Technologies Corporation, where he served as Director of Innovation Business Development (IBD), the Corporate IP monetization organization. He was responsible for patent and technology licensing, patent sales and new business incubation opportunities and was part of the team that built this fledgling organization from concept through over $100 million in committed contract value in three years.
Prior to this role, Suresh was a serial entrepreneur, part of the founding team for four different start-ups, two of which were acquired and one of which is now publicly traded on the Chinese stock exchange.
Suresh also worked at the International Copper Association; at Eastman Kodak Company and at Union Camp Corporation (International Paper) in various process/product commercialization roles as well as served as a Director of the corporate venture capital group at Eastman Kodak.
He holds over 30 U.S. patents and is also a Certified Licensing Professional. Suresh earned his Bachelor of Technology in Chemical Engineering at the Indian Institute of Technology, New Delhi, a Ph.D. in Chemical Engineering at North Carolina State University, Raleigh and an S.M. in Management and Engineering from MIT.

Networking Lunch Kickoff by Justin H.S. Breaux

Justin H. S. Breaux, Digital Communications & External Communications Specialist Communications, Education, and Public Affairs (CEP), Argonne National Laboratory

Justin Breaux writes articles about Argonne's science discoveries and creates posts on social media like Facebook and Twitter to communicate with people outside of Argonne. His job is to let large numbers of people know that Argonne is working on solutions to these global challenges.

Robert G. Sachs Award for Excellence for Outstanding Poster Presentation



Dr. Robert G. Sachs

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

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Poster Abstracts

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Posters Abstracts

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A-1
Ultrafast All-Optical Modulation of Epsilon-Near-Zero Colloidal Nanocrystals

Benjamin T. Diroll,[1] Peijun Guo,[2] Robert P. H. Chang,[2] and Richard D. Schaller[1,3]

[1] Center for Nanoscale Materials, Argonne National Laboratory, Lemont, IL 60439
[2] Department of Materials Science and Engineering, Northwestern University, Evanston, IL 60208
[3] Department of Chemistry, Northwestern University, Evanston, IL 60208

Epsilon-near-zero materials may be synthesized as colloidal nanocrystals which display large magnitude sub-picosecond switching of infrared localized surface plasmon resonances. Such nanocrystals offer a solution-processable, scalable source of tunable metamaterials compatible with arbitrary substrates. Under intraband excitation, these nanocrystals display a red-shift of the plasmon feature arising from the low electron heat capacities and conduction band non-parabolicity of the oxide. Under interband pumping, they show in an ultrafast blueshift of the plasmon resonance due to transient increases in the carrier density. Combined with their high quality factor, large changes in relative transmittance (+86%) and index of refraction (+85%) at modest control fluences (<5 mJ/cm^2), suggest that these materials offer great promise for all-optical switching, wavefront engineering, and beam steering operating at terahertz frequencies.

A-2
Time Resolved Study of Shear-Induced Microstructures of Concentrated Silica Dispersions by SAXS

Jonghun Lee,[1] Xiao-Min Lin,[2] Alec R. Sandy,[1] and Suresh Narayanan[1]

[1] X-ray Science Division, Argonne National Laboratory, Argonne, IL 60439
[2] Center for Nanoscale Materials, Argonne National Laboratory, Argonne, IL 60439

Concentrated colloidal dispersions show non-equilibrium structure formation during shear. These microstructural behaviors affect the macroscopic rheological response. However, there is still a lack of detailed understanding of the link between rheology and microstructure formation, especially regarding the onset of shear thinning and shear thickened/jammed structure. Here, we made simultaneous measurements of rheology and shear-induced structure by small angle x-ray scattering (SAXS) at Sector 8-ID-I of Advanced Photon Source. Concentrated silica dispersions were loaded in Couette cell. The x-ray scattering was measured on velocity-vorticity plane. Under moderate oscillatory shear, particles are rearranged into hexagonal packed layered structures stacking along gradient direction. This rearrangement resulted in reducing the resistance against flow, leading to shear thinning. Upon faster shear, the ordered structure breaks down. But we found that this order-to-disorder transition occurs in a different shear stress regime than the typical shear thickening state, and its occurrence is highly dependent upon oscillatory frequency, particle size and its distribution.

A-3
KAg_3Se_2: Sublattice melting and high electron mobility in a two dimensional semiconductor

Alexander J. E. Rettie,[1] Fei Han,[2] Antia S. Botana,[1] Michael R. Norman,[1] Duck Young Chung,[1] and Mercouri G. Kanatzidis[1,3]

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[2] X-ray Sciences Division, Argonne National Laboratory, Argonne, IL 60439
[3] Department of Chemistry, Northwestern University, Evanston, IL, 60208, USA

Binary silver chalcogenides have long been studied for thermoelectric devices, which recover waste heat as electricity. However, Ag_2S, Ag_2Se and Ag_2Te all undergo superionic phase transitions below 180 °C [1] where the Ag atoms become extremely mobile. Operation above this temperature results in device failure as Ag plates on one electrode. Strategies to push this transition to higher temperatures (or inhibit it completely), while preserving the excellent thermoelectric properties of the silver chalcogenides are therefore of great interest.

One such strategy may be to introduce alkali metal ions into the silver chalcogenides e.g. in the AAg_3Se_2 (A =

K, Rb, Cs) family of compounds. They are isostructural, comprising 2D Ag-Se layers spaced out by the A^+ cations. Although their crystal structures are known, no other material properties have been reported.

Starting with KAg_3Se_2, we show that this material is a narrow band gap semiconductor with a high electron mobility (~500 cm^2 V^{-1} s^{-1} at 300 K) and a high temperature phase transition (on-set: ~700 K) that is consistent with sublattice melting observed in superionic conductors. This transition occurs at a significantly higher temperature compared with the binary silver chalcogenides, and may be linked to the change in crystal structure and unusually low carrier concentration measured in this material.

References
[1] Boyce, J. B. and Huberman, B. A., Superionic conductors: transitions, structures, dynamics. Phys. Lett. Rep., 51, 4 (1979), pp. 189-265.

A-4
Realistic Simulations of the Cosmic Microwave Background

Dr. Samuel Flender (Argonne National Laboratory)

The cosmic microwave background (CMB) is the relic radiation from the Big Bang, and encodes a wealth of information about the early as well as about the late Universe. This poster illustrates some of my work on generating realistic simulations of the CMB, based on the output from state-of-the art cosmological N-body simulations run on the Mira supercomputer at Argonne. The CMB simulations help us obtain a better understanding of the so-called Sunyaev-Zel'dovich (SZ) effect, which is generated by the interactions between CMB photons and the gas residing inside galaxy clusters, the most massive objects in the Universe. The poster illustrates the different types of the SZ effect, and discussed prospects for measuring it with future data.

A-5
Using a new class of peptide-based materials for novel functions

Lee A. Solomon, Matthew Sykes, David Gosztola, Gary Weiderect, and H. Christopher Fry

Center for Nanoscale Materials, Nanophotonics and Biofunctional Structures Group, Argonne, IL 60439

Peptide-Amphiphiles (PAs) are a new material whose functions span many different fields. PA's are composed of a peptide head-group coupled to a lipid tail, and polymerize into various structures depending on the environmental conditions. The sequence of the peptide portion can be amended leading to a range of functions, and to bind biological cofactors. We are interested in the cofactor heme – the same cofactor nature uses to bind gas molecules and transport electrons. Here we show that we are able to control the structure of the peptide, using pH to form either micelles or fibers. We can also induce the formation of sheets using mechanical pressure. We go on to show that the structure and sequence of the peptide segment has a significant effect on heme, changing its ability to take part in oxidation/reduction reactions. Lastly, we take this knowledge and design function into the PA system reproducing natural peroxidase functions –a protein that uses hydrogen peroxide to catalyze the oxidation of small molecules. PA's have significant potential, and the work here shows the first steps toward making functional oxidation catalysts and protein-based wires for environmentally friendly applications.

A-6
Reactive Simulations of the Electrolyte-Electrode Interface in Batteries: Manganese Dissolution and Interfacial Structure

Yasaman Ghadar,[1] Maria K.Y. Chan,[2] and Christopher Knight[1]

[1] Argonne Leadership Computing Facility, Argonne National Laboratory, Lemont, IL, 60439, U.S.A
[2] Center for Nanoscale Materials, Argonne National Laboratory, Lemont, IL, 60439, U.S.A

Lithium ion batteries have been the frontier of energy storage materials for quite some time, making possible

significant advances in mobile consumers electronics and electric vehicles. Under normal operating conditions, side reactions lead to breakdown of the organic electrolyte molecules, resulting in performance loss and safety issues. A fundamental understanding of the key molecular processes taking place at these interfaces is greatly needed in order to help guide the design of new generation batteries.

Reactive molecular simulations of the interface between $LiMn_2O_4$ (001) surfaces and an electrolyte consisting of 1M $LiPF_6$ in ethylene carbonate are used to investigate the critical factors influencing Mn ion dissolution. Free energy profiles for ion dissolution were computed using umbrella sampling calculations for a series of cathodes with varying Li content. These free energy profiles will be compared and correlated with changes in cathode properties, interfacial structure, and system parameters (e.g. temperature) to help develop predictive models for ion dissolution. Additionally, changes in the Mn ion solvation structure will be analyzed utilizing graph theory to understand the electrolyte's role in promoting or inhibiting ion dissolution. The computational performance of the USER-REAXC-OMP package in LAMMPS for these battery systems on IBM BG/Q will also be discussed.

A-7
Real time X-ray Monitoring of Nucleation of AlN on sapphire (0001) during radiofrequency sputtering

Guangxu Ju,[1] Matthew J. Highland,[1] Jeffrey A. Eastman,[1] Rebecca Sichel-Tissot,[1] Peter M. Baldo,[1] Peter Zapol,[1] Hua Zhou,[2] Carol Thompson,[3] and Paul H. Fuoss[1]

[1] Materials Science Division, Argonne National Laboratory, Argonne, IL 60439
[2] Xray Science Division, Argonne National Laboratory, Argonne, IL 60439
[3] Department of Physics, Northern Illinois University, DeKalb IL 60115

We report x-ray scattering studies during growth of AlN nucleation layers on c-plane sapphire via reactive radiofrequency-magnetron sputtering. The sensitivity of these x-ray scattering experiments allowed us to observe the properties of extremely thin nucleation layers and follow the structural evolution of strain and roughness in the AlN layer from an initial nucleation layer to a fully relaxed film. Our results reveal the evolution of the crystal structure, dislocation behavior, and surface and interface roughness during heteroepitaxial growth of a large lattice mismatch system. We observed that threading dislocations were generated once islands coalesced. Misfit dislocations could then glide down into the underlayer to cause residual strain relaxation. $AlN_{1-x}O_x$ formed at the substrate/film interface, and the interface continuously roughened during strain relaxation.

A-8
A high resolution view of air quality from NASA satellites

Daniel L. Goldberg,[1,2] Christopher P. Loughner,[3,4] Lok N. Lamsal,[3] Robert C. Levy,[3] Pawan Gupta,[3] Yang Zhang,[5] Zifeng Lu,[1,2] and David G. Streets[1,2]

[1] Energy Systems Division, Argonne National Laboratory, Argonne, IL 60439
[2] Computation Institute, University of Chicago, Chicago, IL 60637
[3] NASA Goddard Space Flight Center, Greenbelt, MD 20771
[4] Earth System Science Interdisciplinary Center, University of Maryland, College Park, College Park, MD 20742
[5] Department of Marine, Earth, and Atmospheric Sciences, North Carolina State University, Raleigh, NC 27695

Satellite measurements provide greater spatial coverage than any other observing platform, which often makes them advantageous to other measurement techniques. However, due to their large spatial coverage and their usage of monthly mean information from low resolution global models (2.5° × 2°), observations of trace gases (NO_2, SO_2, HCHO, etc.) from satellites have coarse resolution. In this project, we plan to improve the satellite retrieval method by using information from a regional model simulation with horizontal resolution of 1.33 km. Satellite retrievals using this new information will be able to better capture the fine-scale gradients near urban areas and large point sources, which is critical information for those who regulate air pollution, and will further our understanding of the emissions of air pollutants and their subsequent chemical transformations.

A-9
Simulations of Air Flow in a Wind Tunnel

Marta Sitek,[1] Cezary Bojanowski,[1] Steven Lottes[1]

[1] Transportation Research and Analysis Computing Center, Argonne National Laboratory, Argonne, IL 60439

In this research computational fluid dynamics (CFD) was used to perform three-dimensional simulations of the air flow in the Turner-Fairbank Highway Research Center Aerodynamics Laboratory wind tunnel. The computations were performed using high performance clusters available at the Transportation Research and Analysis Computing Center (TRACC) at Argonne National Laboratory. The main goals of the research were to build and verify a detailed model of the wind tunnel and then to propose its simplification, which would make it possible to perform parametric studies with required accuracy, but in less time. The detailed, full-scale model of the laboratory room contained the wind tunnel as well as surrounding furniture and laboratory equipment. Unsteady RANS computations were performed and the rotation of the fan was modeled explicitly. To validate the model, the resulting flow conditions were compared with the lab measurements. An attempt was made to simplify the model, without losing its accuracy, so it is more convenient and time-efficient to run multiple series of tests. In the future the simplified model could provide a valuable tool to perform these types of studies and will be used to complement and extend laboratory experiments.

A-10
Modelling and optimization of solvent drying in electrode processing for battery manufacturing

Naresh Susarla, Shabbir Ahmed, Dennis W. Dees

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The development of efficient and affordable electric vehicles is receiving ever greater interest from both industry and academia. This, indeed, is in the interest of migrating towards emission free vehicles. Arguably, one of the greatest barriers in the successful deployment of electric vehicles is the cost of the batteries inherent to such vehicles. In order to compete with the internal combustion engine (ICE) based vehicles, the current practices of producing the batteries need significant changes in technology and cost. The development of new materials and chemistries for more efficient and economic batteries is receiving a greater interest in the research community. However, for a successful commercialization and to bring down the overall cost, each processing step in the manufacturing of these batteries also needs to be improved and optimized.

Argonne National Laboratory has developed, BatPac, a comprehensive spreadsheet tool for estimating the cost of Lithium Ion Batteries (LIB) with granularity to the cost contribution from each processing step. Analysis of each step, backed by thermal-hydraulic models where possible, offers the potential for quantifying and identifying the opportunities for reducing the cost and energy consumption of each processing step. Among the various processing steps in the production of LIBs, drying and solvent removal from the electrode coating is an energy and cost intensive process [1]. Solvent removal and drying of the coating is also a slow process, which is a potential bottleneck in the production line of LIBs. Thus, it is very useful to study and analyze this processing step in a greater detail. In general, solvent removal and drying has been widely studied [2-4]. However, few studies exist in the literature that focuses on the solvent removal and drying in the context of LIBs. This forms the focus of this study.

In this work, we study and analyze the design aspects and energy requirements of solvent removal and drying in the electrode processing step of LIB production. The heat for the drying is derived from a combination of infra-red (IR) radiators and hot air injectors. We develop a mathematical model of the physical phenomena to understand the various factors affecting the drying rate. The solvent removal involves simultaneous heat and mass transfer with phase change. Our model considers capillary flow and gravity effects for liquid transport and diffusion for vapor phase transport. The model also accounts for the shrinkage of coating thickness with the removal of the solvent and so, the voidage is considered to be a function of solvent saturation in the coating. The system of non-linear partial differential equations is then solved numerically using a finite element method to predict the concentration and temperature profiles within the drying cathode layer. We study the effects of

various factors such as drying temperatures and air conditions on the process performance. Finally, we develop an optimization methodology based on surrogate modelling approach [5] to determine best conditions for electrode drying by minimizing the cost and time.

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A-11

Utilization of a 3D Cell Model in TiO_2 Nanoparticle Mediated Photodynamic Therapy; A Unique Approach in the Pursuit of Colon Cancer Treatment

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- Targeted drug therapies are becoming increasingly utilized for personalized medicine, particularly towards cancer treatments.
- Optimized therapy is based on selectivity and specificity of drug to cancerous tissues.
- We utilize bioluminescence to create light only within the cancer region and in the vicinity of the photoactive TiO_2 nanoparticles.
- We link TiO_2 nanoparticles to firefly Luciferase to create biocomposites that upon activation induce apoptosis in cancer cells.
- TiO_2 biocomposites are 100% effective in 2D *in vitro* studies, but only partially (70%) effective in *in vivo* studies.
- A 3D cell model closely mimics real cancerous tissue, which allows for further optimization of the TiO_2 biocomposite.

A-12

Partition functions for non-rigid molecules

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Accurately modeling chemistry at combustion temperatures requires partition functions that span from 0K to greater than 1000K. Partition functions of non-rigid molecules that undergo large amplitude motions (LAM) are a particularly challenging case as the degree of freedom undergoing LAM is poorly approximated by a harmonic oscillator, even if corrections are made for anharmonicity. A molecule with a single LAM mode can be treated to a good approximation by replacing the harmonic oscillator solution for that single mode with the explicit

solutions of that 1 dimensional potential energy surface. Molecules containing two or more coupled LAM modes require explicit consideration of the potential energy surface containing all LAM degrees of freedoms. A general solution to non-rigid molecules with 2 coupled LAM modes is presented using a discrete variable representation approach1. This approach is in good agreement with previous theoretical and experimental results 2 for hydroxymethyl (CH2OH radical). This work was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences and Biosciences under Contract No. DE-AC02-06CH11357.

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A-13
Numerical Prediction of CCV in SI Engines

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Numerical prediction of cycle-to-cycle variability (CCV) in spark ignition (SI) engines is extremely challenging for two key reasons: (i) high-fidelity methods such as large eddy simulation (LES) are require to accurately capture the in-cylinder turbulent flowfield, and (ii) CCV is experienced over long timescales and hence the simulations need to be performed for hundreds of consecutive cycles. In this study, a new methodology is proposed to dissociate this long time-scale problem into several shorter time-scale problems, considerably reducing the computational time without sacrificing the fidelity of the simulations. The strategy is to perform multiple single-cycle simulations in parallel by effectively perturbing the simulation parameters such as the initial and boundary conditions. This strategy is first demonstrated for a motored engine where the mean and variance of the in-cylinder flowfield is captured reasonably well. The methodology is then extended to a fired PFI SI engine. Here, it is shown that the parallel approach is able to accurately predict the COV of the in-cylinder pressure. It is shown that this new approach is able to give accurate predictions of the flowfield statistics and CCV in less than one-tenth of time required for the conventional approach.

A-14
Computation of the Correlated Metal-Insulator Transition in Vanadium Dioxide Using Quantum Monte Carlo Method

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Vanadium dioxide (VO_2) is a paradigmatic example of a strongly correlated system that undergoes a metal-insulator transition accompanied with a structural distortion. To date, this transition has necessitated significant post-hoc adjustments to theory in order to be described properly. We apply first principles quantum Monte Carlo (QMC) to study the structural dependence of the properties of VO_2. Using this technique, we simulate the interactions between electrons explicitly, which allows for the metal-insulator transition to naturally emerge, importantly without ad-hoc adjustments. The QMC calculations show that the structural transition directly causes the metal-insulator transition and a change in the coupling of vanadium spins. This change in the spin coupling results in a prediction of a momentum-independent magnetic excitation in the insulating state. While two-body correlations are important to set the stage for this transition, they do not change significantly when VO_2 becomes an insulator. These results show that it is now possible to account for electron correlations in a quantitatively accurate way that is also specific to materials.

This presentation is based on our publication: Huihuo Zheng and Lucas K. Wagner, Phys. Rev. Lett. 114, 176401(2015).

A-15
A Combined Experimental and Theoretical Study of the Pyrolysis of 1,3–Butadiene

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Small unsaturated hydrocarbons are important species in combustion chemistry as their thermal decomposition contributes to the radical pool that drives ignition processes. 1,3–butadiene is an archetypal unsaturated hydrocarbon that has been studied extensively using a variety of techniques; yet the exact nature by which the conjugated diene dissociated remains uncertain, with both radical and molecular product paths, as well as isomerization to alternate C_4H_6 species (1,2–butadiene, 1–butyne and 2–butyne) all reported in the literature.

Here we report a detailed study of the thermal decomposition of 1,3–butadiene inside a diaphragmless shock tube using laser schlieren (LS) densitometry to elucidate both the kinetics and mechanism. Experimental density gradient profiles associated with 1,3–butadiene pyrolysis have been measured over a broad range of temperatures (1739 – 2354 K) and pressures (29 – 249 Torr), and a detailed kinetic model has been compiled with the aid of high level theory to simulate all of the experimental density profiles. Both experiment and theory provide strong evidence of a formally direct dissociation path from 1,3–butadiene to $CH_3 + C_3H_3$ products that has not been previously reported in the literature, but which dominates 1,3–butadiene decomposition under the conditions considered here.

A-16
Cooperative Chemical and Structural Transformations in Metal-Organic Frameworks driven by Solvent-Assisted Ligand Exchange

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Metal-organic frameworks (MOFs), with open and ordered porosity, are being pursued as platforms for next generation of designer catalysts. Post-synthetic chemical modifications of MOFs by introducing functional groups into their scaffolds have been a central axis of research, providing routes to developing functionalized frameworks for applications. However, fascinating MOF modifications would arise from combining chemical changes with controllable structural rearrangements on these crystalline materials. Here we show a cooperative chemical and structural transformation occurring on a new microporous framework isomer of the zinc-adeninate framework bio-MOF-100 during post-synthesis modifications (PSM) using Solvent-Assisted Ligand Exchange (SALE). Unlike other MOFs and zeolites, bio-MOF-100 suffers of polymorphism with the less dense phase as final stage. We have used this synthetic tool to prepare the mesoporous bio-MOF-100 functionalized with a molecular iridium catalyst, starting from its pristine microporous analogue. While the structural transformation found in bio-MOF-100-involving a de-interpenetration and a topological transition- is linked to breaking and forming of new bonds, both framework and local structure are preserved.

A-17
Tracking structural changes of layered lithium transition metal oxide electrode over multiple charge-discharge cycles

Hao Liu, Kamila M. Wiaderek, Olaf J. Borkiewicz, Peter J. Chupas, Karena W. Chapman

Layered lithium transition metal oxides are promising high-capacity cathode materials for Li-ion batteries. However, a substantial amount of the theoretical capacity is still not utilized in practice due to rapid capacity

fading when cycled to high voltages, thus limiting its practical use for long-term applications such a grid energy storage. Understanding the structural changes leading to the capacity fade would help us design strategies to alleviate or eliminate this problem. As capacity fading is an accumulative effect that aggravates after each charge-discharge cycle, it would be very difficult to discern the small changes contributing to the capacity fading from a background of more substantial changes due to lithium (de)intercalation. Therefore, it is more beneficial to monitor the structural changes over extended multiple cycles rather than just a few so that trends in structural evolution could be discerned. In this work, we performed in-situ X-ray scattering measurement on a $LiNi_{0.8}Co_{0.15}Al_{0.05}O_2$ electrode to track the structural changes over multiple charge-discharge cycles. Trends in the structural evolution will be discussed in relation to capacity degradation.

A-18
Large-eddy Simulations of Shot-to-shot Variability

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Shot-to-shot variability of fuel sprays is a topic of interest for engine researchers. In particular, how to simulate shot-to-shot variability with modern Computational Fluid Dynamics codes. One method that is easily implemented for Lagrangian spray simulations is to change the random number sequence used to initialize the spray parcels (aka random seed perturbations). This work looks at how well this methodology captures spray variability, and how the predictions are affected by changes in minimum cell size or injected parcel count. Experimental data used for comparison were taken at the Advanced Photon Source at Argonne National Laboratory using a single-hole research diesel injector operating under non-vaporized, high-pressure conditions. Simulations were performed using 3 different minimum mesh sizes (125, 93.75 and 62.5 μm), and 5 injected parcel counts (200, 400k, 600k, 800k, 1200k parcels). 10 Simulation realizations were run for each set-up tested, with time-averaging performed where possible to increase the sample size. Mean quantities were slightly dependent on the minimum cell size, but independent of the injected parcel count. Standard deviations remained constant as a percent of the mean with different minimum cell sizes, but were highly dependent on the number of injected parcels.

A-19
Coarse-grained Modeling of Ultra-thin Nanoparticle Membranes: Effect of Temperature, Humidity, and Ligand Dynamics

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Ultra-thin nanoparticle (NP) membranes can be fabricated via the self-assembly of gold NPs at a liquid-air interface. Dried NP monolayers have high mechanical strength with a surprisingly large Young's modulus on the order of several GPa and can suspend over micron-size holes. NP membranes also have a filtration coefficient for aqueous solutions that is □100 times larger than typical polymer-based membranes. In order to reliably control the large-scale structure and morphology of NP membranes for practical applications such as high-throughput filtration, it is necessary to understand the underlying principles governing the behavior of NP membranes. In our experimental-theoretical study, we looked into the thermo-mechanical properties of NP membranes. Using large-scale coarse-grained molecular dynamics (CGMD) based on the well-known MARTINI force field, we obtained simulation results that are in excellent qualitative agreement with the experimental observations. The simulation trajectories revealed microscopic details, which explained the hysteresis in the Young's modulus curves. The simulations also showed a drop in the Young's modulus when water is present in the membrane, which is consistent with experimental data. Water molecules effectively screen the interactions between NP ligands and also induce their re-organization.

A-20
Structure and stability of LiMO2 (M=Co, Mn, Ni) layered surfaces

Juan Garcia, Javier Bareno, Hakim Iddir

Li ion rechargeable batteries are ubiquitous nowadays at electronic equipment and electric and hybrid vehicles. However, a better cathode material is required to extend the autonomy of such devices. Layered materials as $LiNi_xMn_xCo_{1-2x}O_2$ (NMC) have the potential to have higher energy density and lower costs. However, several drawbacks are still unsolved. For instance, first charge inefficiencies, capacity fading and voltage instability. To overcome these disadvantages a deeper understanding of the processes involved at the molecular level is needed. We modeled at the DFT level NMC cathode materials in order to determine the lowest energy surfaces and the morphology of the crystal particles. We modeled all low index stoichiometric non polar surfaces. Also, we apply simple reconstruction of the top layers to compensate de dipoles on the polar surfaces that we considered. We found that the most stable surfaces are those with the highest coordinated transition metal. Namely the surfaces (001), (-114) and (012) are the most stable and they form the facets of the Wulff construction. Our results match previous experimental results.

A-21
Modeling of Flash Boiling of single component and blended surrogate fuels for Gasoline Direct Injection Applications

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Blending conventional hydrocarbon-based fuels with ethanol is an increasing trend these days to cope with the increment in the green-house gas emissions as well as the depleting fossil fuel reserves. Ethanol contains approximately 33% less energy per unit volume compared to pure gasoline, but higher octane rating of ethanol provides leverage by operating at higher compression ratio (using turbocharger). Increment of ethanol content is one of the directives of Department of Energy (DOE) and Environmental Protection Agency (EPA). The present work involves modeling of internal and near-nozzle flows of a Gasoline Direct Injection (GDI) nozzle using single component (iso-octane and ethanol) and blended (varying % of ethanol by volume) gasoline surrogates. Flash boiling is a common phenomenon in GDI systems, where a high temperature fuel undergoes bulk vaporization in a short span of time when subjected to superheated thermodynamic conditions in the combustion chamber. The current study uses an Eulerian multiphase mixture framework in conjunction with homogenous relaxation model for modeling phase change in pure and blended fuels. A pseudo-single component is used to represent the physical properties of blends (varying proportions of ethanol and iso-octane). The volatility of blended components is sometimes higher than the constituent species due to the inherent non-equilibrium state of the mixture. This strange behavior has led to the prediction of enhanced flashing for specific blends compared to the individual species and the other blends in the current numerical study. The varied levels of flashing tendencies depending on fuel composition therefore, helps in further optimization of spray and combustion research in GDI systems.

A-22
M-to-N Distributed Memory Streaming for In-Transit Data Analysis

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Performing data analysis on intermediate results of a running high-performance computing application has several advantages. It produces an I/O cost savings by performing analysis without the need to write to or read from disk. This in turn enables a higher sampling rate for analysis, which can elucidate complex behaviors

occurring at fine temporal resolution. Additionally, specialized hardware such as high-bandwidth networks and GPUs can be leveraged for analysis at the same time as the CPUs are computing simulation results. The work in this paper focuses on in-transit analysis, where data is streamed from a distributed memory computational resource performing a simulation to a separate distributed memory resource responsible for performing analysis. The main challenge we have addressed is parallel streaming of data between heterogeneous resources running applications that may distribute the data differently. Data is sent from M simulation ranks to N analysis ranks. Data must then be reorganized by the analysis resource to redistribute data from how it was laid out in the simulation application to how it needs to be laid out for the application performing analysis.

A-23

Extreme Scale Quantum Chemistry with Sparse Eigensolvers and Parameterization

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Keywords: High-performance-computing, semi-empirical methods, DFTB, sparse, self-consistent field

Hartree-Fock (HF), density functional theory (DFT) and their parameterized variants such as semi-empirical molecular orbital (SEMO) or tight-binding DFT (DFTB) methods are all based on the self-consistent field (SCF) theory, which generally requires solving an eigenvalue problem many times until a convergence criteria is met. Conventionally, dense linear algebra methods are used to diagonalize the Fock matrix, and this part of the calculation becomes the bottleneck when the matrix size reaches thousands. We have developed and benchmarked a PETSc/SLEPc based sparse eigensolver that makes use of shift-and-invert parallel spectral transformations (SIPs). We demonstrate three main advantages of SIPs compared to dense solvers: 1) SIPs exploits the sparsity of the matrices, hence reduces the memory footprint, and computational complexity 2) SIPs divides the eigenvalue problem into chunks that can be solved independently enabling proven scalability up to hundreds of thousands of cores. 3) SIPs makes use of the eigenvalue distribution at a previous iteration to improve the job balance in the subsequent iteration. We will present benchmark results for the standalone solver for DFTB calculations, SIPs integrated DFT package SIESTA, and a prototype SEMO code that we have developed. Parameterization is important to reduce the computational cost by enhancing sparsity and by eliminating integrals and to obtain useful accuracy for large-scale quantum chemistry calculations. Well-calibrated parameters are required not only for SEMO or DFTB methods, but also for hybrid functionals of DFT. Hence, high-accuracy quantum chemistry calculations are necessary to train parameters for a wide-range of methods. We will present our benchmark results (coupled-cluster calculations at the basis-set limit) for transition metal oxide clusters and their comparison with different DFT functionals.

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A-24
Simulating the Neutrino Sky: Cosmological Probes of Neutrino Mass

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Neutrinos are second only to photons as the most abundant particle in the Universe, yet remain poorly understood due to their weak interaction with other matter. In particular, individual neutrino masses remain an elusive property for both particle physicists and cosmologists. Recently, it has been proposed that individual neutrino mass may be constrained from a unique dipole distortion in the matter density field induced by the relative flow between cold dark matter (CDM) and neutrinos. We study this effect by modifying the cosmology code CUBEP3M to evolve neutrino N-body particles alongside CDM. We have performed the world's largest cosmological N-body simulation, containing roughly 3 trillion neutrino plus CDM particles, completed using 86% of the Tianhe-2 supercomputer. In this poster, we present preliminary analysis of the simulation data in regards to the neutrino dipole distortion. We also present a new independent probe of neutrino mass that was numerically detected in our simulation data. This new effect is caused by neutrino free streaming, which sources local variations in the relative abundance of neutrinos, creating a differential bias that may skew the luminosity function of galaxies.

A-25
Metal Chalcohalide Semiconductors as New Candidates for Room Temperature γ-ray Detector Applications

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A new class of semiconducting compounds including $Pb_7Q_2X_{10}$ and $A_3Bi_2X_9$ (Q = S, Se, Te; A = Rb, Cs; X = Cl, Br, I) known as a ferroelectric family were developed for γ-ray detector applications. The optimization of synthesis, purification and crystal growth to achieve high quality single crystals is presented. This process includes solid state reaction and precipitation in aqueous halides for synthesis, sublimation, bromination, and filtration for purification, and Bridgman technique for crystal growth. Characterization of the materials for crystal structure, optical property, defect analysis, charge transport, photoconductivity, and γ-ray spectroscopy are discussed.

A-26
Circular Dichroism of Angular Distributions (CDAD) by Using Velocity Map Photoelectron Imaging

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Photoelectron angular distributions (PAD) recorded following ionization with polarized light can be used to probe the orientation and alignment of excited atoms and molecules, and provide insight into the details of the photoionization dynamics.[1] In particular, the circular dichroism of photoelectron angular distributions (CDAD) can be used to perform "complete" photoionization experiments, allowing the extraction of all of the dynamical parameters required to describe the process. In CDAD experiments performed before the development of VMI, a linear polarized pump beam was followed by a left- or right circular polarized probe beam, and the difference in signal for the two circular polarized beams was monitored as a function of the angle between the pump polarization and the detection angle. The resulting experiments require photoelectron spectra at many angles, and are time consuming. Here we explore the possibility of using a circular polarized pump beam and left and right circular polarized probe beams, along with VMI along the axis perpendicular to the laser propagation axes. We have employed this technique to study the (1+1') photoionization of NO. Our results are compared with theoretical CDAD spectra calculated by using the previously determined dynamical parameters.

[1] K.L. Reid Annual Review of Physical Chemistry 2003 Vol. 54: 397-424.

A-27
The Three-Dimensional Structure of the Barite (001)-Water Interface

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The three-dimensional structure of the barite (001)-water interface has been determined using high-resolution X-ray reflectivity measurements. Ten crystal truncation rods were measured, which provide both lateral and vertical sensitivity to the structure of the barite-water interface. The results demonstrate that there are two interfacial water layers with heights of 2.2 ± 0.2 and 3.3 ± 0.2 Å from the Ba ions at the top surface. The water molecules in these two layers are coordinated with both the barium and sulfates at the surface. We also find that the barium and sulfate atoms at the surface shift laterally (by ≤0.15 Å) and vertically (by ≤0.12 Å), with relaxations occurring up to three unit cells deep into the sub-surface. The largest displacements are observed in the top unit-cell layer, with an increasingly uniform coordination geometry occurring further into the crystal. Small rotations (< 3°) of the surface sulfate molecules are also needed to explain the XR data. Overall, our results show a good agreement with those from a previous specular XR study [1] in terms of the trend observed in the vertical structural changes, and also provide new insights into the lateral structural changes. These results are also consistent with those from previous molecular dynamics (MD) simulations [2] although the vertical distributions of adsorbed water molecules in the MD simulations were more diffuse than those determined by the present XR data.

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A-28
Uncertainty Quantification of Nuclear Reactor Safety with SAS4A/SASSYS-1 and DAKOTA

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Advancements in the knowledge of nuclear reactor performance have led to an increased need to perform Uncertainty Quantification (UQ) in the advanced reactor domain. The role of uncertainty quantification spans many facets in the nuclear industry, including system design and optimization, licensing, and probabilistic risk assessment. The objective of this study is to apply the recently developed coupling between Dakota and Argonne nuclear reactor safety software, called SAS4A/SASSYS-1, to investigate the impact of uncertainties on the simulation results. The Dakota software is an uncertainty quantification and optimization toolkit and was coupled with SAS4A/SASSYS-1 via a Python interface. Dakota was used to sample user-specified parameters, drive SAS4A/SASSYS-1 transient simulations, and quantify statistical metrics as part of post processing. The toolkit was applied for the uncertainty quantification of the Experimental Breeder Reactor II (EBR-II) Balance-of-Plant (BOP) tests that represented protected and unprotected loss of heat sink conditions. Some assumptions had to be made for the models because of uncertainties related to the cooling system. In addition, the reactivity feedback coefficients also have uncertainties due to the nuclear data. These uncertainties may contribute to discrepancies observed between the simulation results and the measured data. The studies include the uncertainty quantification of the EBR-II simulations and the calibration between the simulation results and the experimental data. By applying Dakota for uncertainty propagation, it is found that the radial expansion, the control rod drive expansion, and the stagnant sodium mixing models have significant impacts on the benchmark results. Following the uncertainty quantification, parameters in the EBR-II model that were identified to have significant impacts were optimized by Dakota in order to improve the agreement between the simulation results and the measurements.

A-29
Topology-Aware Data Aggregation for Intensive I/O on Large-Scale Supercomputers

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Reading and writing data efficiently from storage systems is critical for high performance data-centric applications. These I/O systems are being increasingly characterized by complex topologies and deeper memory hierarchies. Effective parallel I/O solutions are needed to scale applications on current and future supercomputers. Data aggregation is an efficient approach consisting of electing some processes in charge of aggregating data from a set of neighbors and writing the aggregated data into storage. Thus, the bandwidth use can be optimized while the contention is reduced. In this work, we take into account the network topology for mapping aggregators and we propose an optimized buffering system in order to reduce the aggregation cost. We validate our approach, on micro-benchmarks and the cosmological application HACC. We show improvements up to 15× faster for I/O operations compared to a standard implementation of MPI I/O.

A-30
Advanced Oil Sorbents

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Disasters on the scale of the Exxon Valdez and Deepwater Horizon serve as harrowing reminders of the devastating effects uncontrolled oil spills have on the environment. Skimming, burning, and dispersing oil are only partially effective and carry their own ecological impacts. An enticing alternative strategy involves oil sorbents capable of efficient extraction of oil from water bodies, which in turn necessitates the design and implementation of novel materials. Here, I will describe our most recent attempts to do so by targeting superoleophilic and superhydrophobic chemistries. Using these results, we are able to outline an effective design principle for new classes of oil sorbents for oil spill remediation, and demonstrate sorption coefficients on the order of 30 g/g for crude oil in model seawater.

A-31
First-Principles Studies of Earth-Abundant Thermoelectrics

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Thermoelectric material is an alternative renewable energy technology for waste heat recovery. Its efficiency is characterized by the 'dimensionless figure of merit' *ZT*, we identify promising candidates among bulk compounds with earth-abundant elements (particularly minerals) via first-principles calculations of electronic and thermal transport properties. Our recently developed compressive sensing lattice dynamics (CSLD) method allows us to calculate low lattice thermal conductivity in strongly anharmonic crystals and identify the impact of nanostructuring and alloying on reducing lattice thermal conductivity. One of our predicted (also experimentally synthesized) minerals, tetrahedrite ($Cu_{12}Sb_4S_{13}$) has achieved ZT~1.0 and been put into commercial product due to its wide availability, easy and rapid synthesis routine.

B-1
Fragment Approach to Density Functional Theory Calculations of Large Systems

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Density-functional theory (DFT) has become the dominant method for electronic structure simulations due to its excellent balance between accuracy and efficiency. However, standard implementations of DFT scale cubically with the number of atoms and so reduced scaling algorithms are required to allow simulations of realistic (large) systems of technological importance. To this end, a linear-scaling approach has recently been implemented in BigDFT, wherein a minimal set of localized support functions are expressed in an underlying wavelet basis and optimized to reflect their chemical environment. This not only allows the treatment of tens of thousands of atoms, but also facilitates the straightforward definition of a fragment approach, which reduces the computational cost by up to an order of magnitude while also offering additional flexibility. Such an approach has previously been applied to supramolecular systems, where it was shown to be effective in treating environmental effects within

the context of constrained DFT. An embedded fragment approach has also now been developed for extended systems, which is particularly suited to the treatment of defective materials. We will describe the BigDFT fragment approach and present examples of its application to both molecular and extended systems.

B-2
Employing Black Silicon in Bio Applications

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Novel nanomaterials are being used increasingly in medical applications. Accompanying this growth in importance is a strong need for protecting these unique surfaces from individual microorganisms and mixtures of organisms that can form biofilms - coatings that can potentially render the approaches harmful to patients.

In this study, black silicon, exhibiting a nanoscale topology containing surface spikes with dimensions and spacings similar to that of the waxy protrusions on insect wings, has been fabricated, materials properties characterized and bactericidal properties investigated. Black silicon was produced via a self-masking, lithography-free reactive-ion etching technique. We show how the nanotoplogy (pillar length, diameter, shape, spacing and uniformity) of the material can be varied with controlled modification of the etching conditions. The interaction of these materials with bacteria possessing differences in the thickness and composition of cell walls and outer membranes was studied in detail. Variables shown to be important for bactericidal efficacy include – but are not limited to – temperature, the ratio of the number of spikes per cell, and the density of spikes on the materials surface. Experiments were conducted by comparing the number of viable cells (those able to form colonies on an agar plate) after incubation of bacteria. The bactericidal effect has been confirmed for all bacteria types studied. Incorporation of these types of surfaces may prove to be important design considerations in medical applications using abiotic components.

B-3
Thermal Transport Across Metal Silicide-Silicon Interfaces: First-Principles Calculations and Green's Function Transport Simulations

Sridhar Sadasivam

Heat transfer across metal-semiconductor interfaces involves multiple fundamentaltransport mechanisms such as elastic and inelastic phonon scattering, and electron-phonon coupling within the metal and across the interface. The relativecontributions of these different transport mechanisms to interface conductanceremains unclear in the current literature. In this work, we use a combination of first-principles calculations under the density functional theory framework and heattransport simulations using the atomistic Green's function (AGF) method toquantitatively predict the contribution of the different scattering mechanisms to thethermal interface conductance of epitaxial CoSi2-Si interfaces. An importantdevelopment in the present work is the direct computation of interfacial bondingfrom density functional perturbation theory (DFPT) and hence the avoidance ofcommonly used `mixing rules' to obtain the cross-interface force constants frombulk material force constants. Another important algorithmic development is theintegration of the recursive Green's function (RGF) method with Büttiker probescattering that enables computationally efficient simulations of inelastic phononscattering and its contribution to the thermal interface conductance. First-principlescalculations of electron-phonon coupling reveal that cross-interface energy transferbetween metal electrons and atomic vibrations in the semiconductor is mediated bydelocalized acoustic phonon modes that extend on both sides of the interface, andphonon modes that are localized inside the semiconductor region of the interfaceexhibit negligible coupling with electrons in the metal. We also provide a directcomparison between simulation predictions and experimental measurements ofthermal interface conductance of epitaxial CoSi2-Si interfaces using the time-domainthermoreflectance technique. Importantly, the experimental results, performedacross a wide temperature range, only agree well with predictions that include alltransport processes: elastic and inelastic phonon scattering,

electron-phononcoupling in the metal, and electron-phonon coupling across the interface.

B-4

Mesoscale model for fission-induced recrystallization in U-7Mo alloy

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A mesoscale model is developed by integrating the rate theory and phase-field models and is used to study the fission-induced recrystallization in U-7Mo alloy. The rate theory model is used to predict the dislocation density and density of the recrystallized nuclei due to irradiation. The predicted fission rate and temperature dependences of the dislocation density are in good agreement with experimental measurements. This information is used as input for the multiphase phase-field model to investigate the fission-induced recrystallization kinetics. The simulated recrystallization volume fraction and bubble-induced swelling agree well with experimental data. The effects of the fission rate, initial grain size, and grain morphology on the recrystallization kinetics are discussed based on an analysis of recrystallization growth rate using the modified Avrami equation. We conclude that the initial microstructure of the U-Mo fuels, especially the grain size, can be used to effectively control the rate of fission-induced recrystallization and therefore swelling.

B-5

Catalysis at a Subnanometer Scale: Tuning Activity and Selectivity

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Nanoclusters comprised of a handful of atoms can exhibit catalytic properties not observed in their bulk analogues, due to the availability of maximal active sites[1,2,3].

We developed a novel catalytic system by depositing monodispersed palladium clusters, Pd_n (n = 4, 5, 8) on ultrananocrystalline diamond (UNCD) supports for oxidative dehydrogenation of cyclohexane. The reaction is of prime importance in chemical industry for e.g. benzene production, but requires a high temperature resulting in undesired CO_2 release. Our results show benzene formation with high activity and selectivity at temperatures as low as 200 C. *In situ* grazing-incidence small angle X-ray scattering show that clusters is stable against agglomeration, which is important for applications. X-ray absorption spectroscopy reveals that the active phase of clusters is metallic. Strong cluster size and support dependence is observed when comparing UNCD and currently used titania and alumina supports. Studies performed with Cu_n (n = 4, 5, 12, 20) clusters on UNCD and alumina supports demonstrated different selectivity, yielding important intermediate products such as cyclohexene and cyclohexanone. The new materials offer an excellent approach for tuning activity and selectivity. By optimizing cluster size, composition, and choice of support the most cost efficient catalyst can be developed.

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B-6
Characterization of the relationship between application I/O time and system-wide I/O traffic on leadership-class computing systems

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The complexity of leadership-class computing storage systems presents extreme challenges in making best use of limited I/O resources. System modeling can be used to better understand I/O behavior on these systems and to utilize I/O resources more efficiently. To this end, we developed a systematic statistical/machine learning methodology to study the relationship between I/O time of applications measured using Darshan [1] and system-wide I/O as measured using iostat [2] as the aggregate read and write bandwidth to the storage at a sixty second granularity.

We apply this methodology to data obtained on leadership-class computing system over a two-month period. Our results show that there is a positive correlation between observed I/O time and system wide I/O for most of the applications. Also, we found that keeping track of the read and write bandwidth separately gives a richer insight than their linear combination. In addition, the conditional distribution of I/O time confirms the positive correlation as well as shows that the credible intervals on I/O time do not vary significantly with change in system-wide I/O. This methodology allows us to gain a deeper understanding of the influence of system state on the application run time, which could be used to enhance scheduling optimizations as well as application I/O strategies, system software optimizations, and system architectures.

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B-7
Ultra-broadband Hot Electron Response in a Plasmonic Metasurface

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Upon photoexcitation in plasmonic metallic nanostructures, surface plasmons rapidly decay to produce hot electrons near the metal's surface through intra- or interband transitions. These charge carriers initially form a nonthermal energy distribution and have been theorized to exhibit a range of relaxation times on the order of 10 - 100 fs. Using transient absorption spectroscopy, we resolve the spectral and temporal response of both nonthermal and thermal hot electrons excited in a plasmonic metasurface comprising substrate-coupled silver nanocubes in a nanopatch antenna geometry. The ultrafast, ~100 fs spectral response from hot electrons is shown to extend over 1000 nm from the ultraviolet to near-infrared wavelengths due to the perturbation of multiple plasmonic and interband transitions of the metasurface. Through experiment and modeling, we describe how both nonthermal and thermal carriers couple to the various optical modes and show opposite spectral signatures for the two electron populations. The ultrafast response demonstrated here occurs at the limit of the electronic response in metals, potentially enabling THz switching of optical signals from the infrared through UV, advancements in photocatalysis and photodetectors, and nonthermal systems far from equilibrium.

B-8
Characterizing evolving processes through coupled CDI and molecular dynamics studies

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Coherent X-ray diffraction imaging (CDI) is a powerful technique for operando characterization with the ability to provide time-evolving snapshots of defect structure, lattice dynamics and structural changes. It is however, limited to ~10 nm in spatial resolution, and can only image crystalline structures. Molecular dynamics (MD) simulations provide a complete atomic picture of dynamically evolving processes for system sizes that perfectly complement CDI experiments. Integrating the two approaches can provide insights into the underlying physics of materials processes that go beyond what each technique individually is capable of. Case studies from recent joint experimental and modelling studies of slowly evolving, catalytic processes as well as ultra-fast lattice dynamics following laser excitation will be presented. Finally, we look at the potential to extend the effective resolution provided by CDI by coupling molecular statics (MS) simulations to experimental data through machine learning approaches.

B-9
Structure and Electrochemical Behavior of Cerium Polynuclear Clusters

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Unique among the lanthanides, cerium can exist in aqueous solutions as a tetravalent cation (Ce^{IV}), which can readily hydrolyze and condense to form polynuclear clusters and the well-known catalyst, ceria (CeO_2). Examining discrete Ce^{IV} polynuclear clusters can provide insight into the underlying electronic and structural influences driving aqueous Ce^{IV} chemistry and the catalytic behavior of nanosized CeO_2. Here, we report the isolation, structural characterization via single-crystal X-ray diffraction, and redox behavior of dinuclear and hexanuclear Ce^{IV} clusters. Synthesized from acidic nitrate solutions, these clusters are decorated by nitrate, water, and, glycine (hexanuclear cluster only) ligands. Cyclic and differential voltammetry for the dinuclear cluster, which contains a unique linear μ-oxo bridge not found in other tetravalent metal (M^{IV}) dinuclear clusters, indicate stabilization of Ce^{IV} within the dinuclear cluster relative to the monomeric Ce^{IV} aquo ion. In the hexanuclear cluster, voltammetry indicates that Ce^{IV} is more stabilized than in the dinuclear cluster, suggesting that the stability of Ce^{IV} increases as cluster nuclearity increases. Together, these findings provide insight into the formation, structure, and stability of Ce^{IV} polynuclear clusters. This work was performed at Argonne National Laboratory, operated by UChicagoArgonne LLC, and supported by the U.S. DOE BES, Heavy Element Chemistry Program (DE-AC02-06CH11357).

B-10
Progress Towards Dichroic Bragg Coherent Diffractive Imaging

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Magnetization is coupled to the atomic lattice strain in crystals by the magnetoelastic energy. X-ray diffraction methods are powerful tools for study of magnetism and lattice strain, however there are currently no tools for measuring these properties simultaneously at the nanoscale, where local strain fields can influence magnetic domain configurations. By combining x-ray magnetic circular dichroism and Bragg coherent diffractive imaging

methods, it should be possible to image nanoscale strain and magnetization at the same time, with a single measurement. We are developing dichroic BCDI techniques for imaging strain and magnetization simultaneously, in two and three dimensions, in isolated magnetic nanocrystals as well as magnetic thin films. We use circularly polarized x-rays produced by a diamond x-ray phase retarder to gain sensitivity to magnetism. To quantify the feasibility of these methods we are testing them with novel magnetic material systems such as faceted Cobalt-Platinum nanocrystals and tungsten-encapsulated Gadolinium nanocrystals.

B-11
Disproportionation in spinel lithium manganese oxide from first principles

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Spinel lithium manganese oxide (LMO) is a promising cathode material in Li-ion batteries, however, dissolution of manganese from LMO to the electrolyte limits its cycle life. Although it is believed that dissolution of manganese is a result of a disproportionation reaction, the atomistic details of such a process remained elusive. Here, we look at disproportionation in bulk LMO using first principles methods and discuss the structural and electronic properties of LMO before and after disproportionation.

B-12
Molecular-Scale Investigation Of Anion Adsorption Competition At A Charged Langmuir Monolayer

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Competitive ionic adsorption at charged interfaces occurs abundantly in natural and industrial processes, including heavy metal separations. However, very little is known about the interactions that drive preferential ionic adsorption at charged interfaces. We studied the competition between divalent chlorometallate anions ($PtCl_6^{2-}$ and $PdCl_4^{2-}$) and monovalent chloride anions at positively charged Langmuir monolayers using specular X-ray reflectivity (XR), grazing incidence X-ray diffraction (GID), X-ray fluorescence near total reflection (XFNTR), and vibrational sum frequency generation (VSFG) spectroscopy.

Molecular vibrations are only VSFG-active if there is a break in inversion symmetry. Bulk media is symmetric, but symmetry is broken at an interface, so VSFG is inherently surfacespecific. Here, we use VSFG to probe the interfacial water structure at the water-ion-surfactant interface. Charged interfaces induce extended water order, which leads to strong water VSFG signal; the addition of ions forms an electric double-layer, reducing the effective charge on the interfacial water, which suppresses the water VSFG signal. In the presence of heavy metal ions, we observe a new peak from weakly interacting water. The presence of this peak likely indicates that water is trapped near the surfactant between the positive headgroups and nonpolar tails.

B-13
Efficiency of Electricity Markets: Impact of Network Topology and Uncertainty

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We study the robust supply function equilibrium (SFE) in deregulated electricity markets.Specifically, we consider a market where the energy suppliers submit their supplyfunctions and bid to fulfill an inelastic demand. Suppliers have renewable energygeneration (with zero marginal cost) and conventional energy generation (with variablemarginal costs). Each supplier performs robust optimization against the worst-caserealizations of its renewable energy generation and opponents' marginal costs ofconventional energy generation. We analyze the

resulting robust SFE and its efficiency.

B-14

Minimizing Microbial Community Complexity for Annotating Metabolic Signaling Networks Over Time: Understanding How Microorganisms Communicate in a Dynamic Environment

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The application of engineered microbial populations for environmental or therapeutic manipulation is contingent upon understanding the mechanisms required for their stability and persistence over time. Growth dynamics of *a priori* defined low-complexity systems (i.e. synthetic communities) have been studied but few examples exist derived directly from naturally-occurring communities (e.g. soil). In this work, we are focused on identifying key interactions responsible for intermediate community stability by isolating and studying what we term "minimal communities" via a high-throughput substrate screening and cultivation platform. Samples are then grown in parallelized continuous cultivation to test perturbations in response to abiotic stressors – for example, pH. As a primary selective pressure shown to affect community composition, pH perturbations will enable us to ultimately study how secondary metabolites differ between community subsets. Sub-communities were cultured in a low volume (<20 mL) continuous culture system for temporal analysis by a mass spectrometry-based metabolomics screening approach and subsequently 16S rRNA-based amplicon sequencing. Understanding of this microbial language is in its infancy but we believe it can be simplified within the context of minimal communities for the establishment of metabolic models that can be leveraged for community engineering.

B-15

Recombination and Dissociation of 2-Methyl Allyl Radicals: Experiment and Theory

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Resonantly stabilized radicals (RSRs) are a key class of species in combustion systems and are typically much less reactive than other combustion radicals such as OH, H, and O. Consequently, RSRs can accumulate in relatively large concentrations and significantly affect combustion chemistry. For example, the 2-methyl allyl radical (2-MA) plays an important role in the low temperature ignition of isobutene and is responsible for the effectiveness of tert-butyl ethers in suppressing engine knock. Accurate rate constants for reactions involving 2-MA at a broad range of temperatures and pressures are necessary for chemical kinetic modeling of combustion systems.

A combined experimental and theoretical investigation of 2-MA was conducted to determine rate constants for dissociation and recombination of 2-MA. Experiments were conducted in a diaphragmless shock tube in the temperature range 724-1336 K using two different precursors: 3-methylbut-3-enyl nitrite (724 K < T < 1061 K) and 2,5-dimethyl-1,5-hexadiene (1090 K < T < 1336 K) as thermal precursors of 2-MA. The experiments are complemented by *a priori* theoretical calculations for both the recombination and dissociation of 2-methylallyl, and the experimental results and theoretical predictions are in excellent agreement with one another.

B-16
Degenerate, Open Shell Density Perturbation Theory

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Fractional occupation numbers can be used in density functional theory to create a symmetric Kohn-Sham potential, resulting in orbitals with degenerate eigenvalues. We develop the corresponding perturbation theory and apply it to a system of Nd degenerate electrons in a harmonic oscillator potential. The order-by-order expansions of both the fractional occupation numbers and unitary transformations within the degenerate subspace are determined by the requirement that a differentiable map exists connecting the initial and perturbed states. Using the Xα exchange-correlation (XC) functional, we find an analytic solution for the first-order density and first through third-order energies as a function of α, with and without a selfinteraction correction. The fact that the XC Hessian is not positive definite plays an important role in the behavior of the occupation numbers.

B-17
Shallow And Deep Traps In Quantum Dot Solids

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Defects in semiconductor quantum dot (QD) solids are commonly believed to be the main cause for the poor charge transport properties of QD devices[1,2,3]. However, atomistic details of how defects slow down charge transport or trap charges are poorly understood. We explored hopping transport in silicon QDs with two common defects: dangling bonds and oxygen impurities. While dangling bonds are thought to be the primary cause of poor transport in Si QDs, we found that shallow defect states (from oxygen) can be even more detrimental to transport than deep defect states (dangling bonds). In some scenarios, oxygen defects trap electrons two orders of magnitude faster than dangling bonds. This counter-intuitive result highlights the importance of atomistic details for the transport properties of QDs and suggests that the defect state energies are insufficient to predict trapping rates. Finally, a new methodology for modeling charge transport near electrode and substrate surfaces is developed, and we describe conditions for when significant changes occur near surfaces.

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B-18
Towards Predictive Simulation of Ignition Events in Gasoline Engines

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Study of ignition fundamentals has gaining research interests over the recent decade as a result of pursuing higher thermal efficiency in gasoline engines. Lean and/or dilute combustion is believed to deliver improved fuel economy while increased cyclic variability also rises as a side effect. The duration of early flame development has been found to vary more significantly than the rest of the combustion process under challenging conditions, which leads to the necessity to investigate and improve the ignition process. This numerical study aims to develop comprehensive simulation tools to assess ignition systems' effects on early flame development. Close

collaboration has been established with experimentalists to better understand the characteristics of various ignition technologies ranging from conventional spark to advanced non-equilibrium plasma systems. A detailed numerical framework has been established and yielded promising results for conventional systems. Future research will focus on extending the capability of this simulation tool to assist the design and development of future ignition technologies.

B-19

CFD Simulation Of A Multi-Hole Diesel Injector With Naphtha Fuels On Varying Operating Conditions, Mesh Motion And Refinement Strategies

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The influence of fuel properties and the understanding of injection processes are two of many aspects commonly addressed when investigating Internal Combustion Engines (ICE). In this work, previously validated methodologies were adapted to the use of two new gasolinelike fuels, full-range naphtha and light naphtha. Previous studies with n-dodecane showed that the characteristics of internal and near nozzle flow were strongly related to the needle motion. Furthermore, physical properties of the fuel like density, viscosity and saturation pressure were fundamental in defining the way mass enters the chamber, its injected amount and the possibility of cavitation. Here, these aspects were evaluated on varying needle motion characteristics, domain discretization, geometry details and injector operating conditions. Simulations were carried out in the commercial code CONVERGE, using a fully compressible multi-phase solver based on the mixture model assumption with Volume Of Fluid (VOF) method. The investigation was performed by comparing mass flow rates and area contraction coefficients at the nozzle outlets, and local distributions of gas volume fraction, velocity and pressure within the nozzles. Mesh embedded refinements in the near-nozzle area were also discussed in order to evaluate their influence on the in-nozzle flow. As a result, their exclusion for reducing computational effort without losing accuracy was assessed. Finally, the comparison between baseline conditions and additional cases was provided to show qualitative and quantitative predictions for the adopted fuels.

B-20

Assessing The Contribution Of DNA Methylation To Primate Regulatory Evolution

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Gene regulation has long been thought to be a driving force in adaptive evolution. Despite evidence that regulatory changes contribute to many species-specific adaptations, the mechanisms of regulatory evolution remain elusive. We leverage inter-tissue and inter-species comparisons to determine the contribution of DNA methylation changes to the evolution of gene expression.

We assessed CpG methylation status across the genome by performing whole-genome bisulfite conversion followed by high-throughput sequencing across 4 tissues (heart, kidney, liver and lung) in human, chimpanzee, and macaque samples. We collected gene expression profiles from the same samples, allowing us to perform a high resolution scan for genes and pathways whose regulation evolved under selection. By integrating these

methylation and expression datasets, we characterized the genomic features where methylation most contributes to expression changes. To understand how epigenetic divergence contributes to gene expression evolution, we modeled the proportion of variation in gene expression levels across tissues and species explained by changes in methylation. We discovered strong negative associations between gene expression and methylation changes across tissues but greatly reduced correlations across species. This may imply that changes in epigenetic regulation are generally not a causal mechanism of primate evolution.

B-21
Spin Dynamics of Artificial Spin-Ice Systems

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Frustrated magnetic systems, such as spin ices, have been of interest for a long time. Artificially structured spin ices offer the opportunity to engineer interactions between elements. However, up until now, there are only few works on artificial spin-ices reported in the GHz-regime.

Here, we present results on spin dynamics of spin-ice lattices made of $Ni_{80}Fe_{20}$ [1]. The samples were fabricated by electron beam lithography and we use broadband ferromagnetic resonance spectroscopy to study the dynamics. An excellent qualitative agreement of the experimental mode spectra to a semianalytical model is found. Furthermore, a hysteretic behavior of modes in the low field regime is observed, which we correlate with the magnetization states of individual islands. Our results are first steps towards the understanding of artificial geometrically frustrated magnetic systems in the GHz-regime.

Furthermore, we explore the possibility to detect spin dynamics in $Ni_{80}Fe_{20}$/Pt antidote lattices, which can be considered as interconnected spin-ice systems, by pure dc electrical means [2].

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References:
[1] M. B. Jungfleisch et al., Phys. Rev. B 93, 100401(R) (2016).
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B-22
PICS: SIMULATIONS OF STRONG GRAVITATIONAL LENSING IN GALAXYCLUSTERS

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Cosmological strong gravitational lensing, in particular, probes the properties of the densecores of dark matter halos over decades in mass and offers the opportunity to study thedistant universe at flux levels and spatial resolutions otherwise unavailable. One of thechallenges in realizing the potential of strong lensing is to understand the statistical contextof both the individual systems that receive extensive follow-up study.

Motivated by thesechallenges, we have developed an image- simulation pipeline, PICS (Pipeline for Images ofCosmological Strong lensing) to generate realistic strong gravitational lensing signals fromgroup- and cluster-scale lenses. Lensed images are produced by ray-tracing images ofactual galaxies from deep Hubble Space Telescope observations. Other galaxies, similarlysampled, are added to fill in the light cone. The pipeline further adds cluster-membergalaxies and foreground stars into the lensed images. The entire image ensemble is thenobserved using a realistic point spread function which includes appropriate detectorartifacts for bright stars. Noise is further added, including such non-Gaussian elements asnoise window-panning from mosaiced observations, residual bad pixels, and cosmic rays.The aim is to produced simulated images that appear identical—to human's eyes—to realobservations in various imaging surveys.

B-23
An Agent Based Model Of Spread Of Competing Rumors Through Online Interactions On Social Media

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The continued popularity of social media in the dissemination of ideas and the unique features of that channel create important research opportunities in the study of rumor contagion. Using an agent-based modeling framework, we study agent behavior in the spread of competing rumors through an endogenous costly exercise of measured networked interactions whereby agents update their position, opinion or belief with respect to a rumor, and attempt to influence peers through interactions, uniquely shaping group behavior in the spread of rumors. It should be pointed out that this research is still in its nascent stages and much needs to be further investigated. Our initial findings, however, suggest that (i) rumors can survive under competition even with low adopting populations, (ii) latent positions in rumors seem to dominate extreme positions, and (iii) the timing of the effort expended by an agent affects the level of competition between rumors.

B-24
Performance of 2G-HTS undulator coils secured with epoxy components

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Undulator magnetic structures using second-generation high temperature superconducting (2G-HTS) tapes have been recently evaluated and shown to be viable with superior performance. Securing the tape mechanically and providing enough conduction cooling to the winding stacks remain challenging problems. In this study, we have used epoxy impregnation techniques to address these issues. We have also investigated the effect of epoxy on the performance of the undulator coil pack. The results showed that epoxy component cannot be used alone and to prevent the performance degradation either the epoxy thickness needs to be reduced or a bumper layer between the coil and the epoxy needs to be introduced. Microstructures also revealed that vacuum impregnated coil pack has a more uniform winding layers and less epoxy between the layers, which is important for the overall performance of the device.

B-25
The Use of an Energy Criteria to Predict White Etching Crack Formation in Bearing Steel

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White etching cracks (WECs) have been identified as a dominant mode of premature failure within wind turbine gearbox bearings. Though WECs have been reported in the field for over a decade, the conditions leading to

WECs, and the process by which this failure culminate, are both highly debated. In previously published work, the generation of WECs on a bench top scale was linked to sliding at the surface of the test sample, it was also postulated that the generation of WECs was dependent on the cumulative energy that had been applied to the sample over the entirety of the test. In this paper, a three ring on roller bench top test rig is used to systematically alter the cumulative energy that a sample experiences through changes in normal load, sliding, and run time, in an attempt to correlate cumulative energy with the formation of WECs. It was determined that, in the current test setup, the presence of WECs can be predicted by this energy criterion. The authors then used this information to study the process by which WECs initiate. It was found that, under the current testing conditions, the formation of a dark etching microstructure precedes the formation of a crack, and a crack precedes the formation of white etching microstructure.

B-26

Designing Nanostructured Mixes Heusler Systems For Improved Thermoelectrics

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The search for new and more efficient thermoelectric materials has been gathering a large momentum, with a special attention focusing on the improvement of the ZT by forming nanostructures in a host matrix. Particular interest has been directed to the Heusler compounds, especially due to their favorable electrical properties and the possibility of lowering their thermal conductivity via introducing nanostructures. Our study aims in predicting the possibility of forming nanostructured systems between full and half Heusler host matrices with other Heusler compounds (half, inverse and full Heusler), using density functional theory calculations. Our prediction is based on estimating the solvus between the two Heusler compounds, the matrix and the nanostructured compound, using the mixing energy and considering the pairs within a mixing energy interval that favors nanostructuring. Screening the Heusler pairs using this approach gave25 matrix/nanostructured compound pairs that have not been previously considered as nanostructured thermoelectrics. In addition, based on the mixing energies we argue that different types of Heusler compounds, e.g. half and full Heusler, would favor formation of stable interfaces with low intermixing between the phases, and Heusler compounds of the same type would form nanocomposites or solid solutions.

B-27

Development Of Tabulated Combustion Models For Faster CFD Simulations

Prithwish Kundu, Muhsin Ameen, Sibendu Som

Materials Energy Systems, Argonne National Laboratory

Stiff chemistry of large mechanisms and resolution of small time and length scales have been the main bottlenecks towards predictive modeling of engines. This work develops a novel flamelet tabulation technique, which has demonstrated significant speed up compared to the existing combustion models. The validations were carried out over a range of conditions against lab experiments as well as engines. The improved models have led to reduced costs as well as provided new insights into fundamentals of combustion. Low temperature combustion regimes are the future of engine technology. These scenarios of reacting spray flames were simulated using the new models to gain insights in auto-ignition and flame stabilization processes, which was not possible previously. Further development will enable CFD models to include detailed chemistry with thousands of species along with high-resolution grids. These developments will eventually push CFD models to become more predictive and help engineers design better engines.

B-28

Premature Mitotic Activation Inhibits Pseudo-Bipolar Spindleformation And Tumor Growth

Amitabha Mukhopadhyay[¶, 1], **Lalit Sehgal**[1], **Arunabha Bose**[1], **Anushree Gulvady**[1], **Parijat Senapati**[4], **Rahul Thorat**[1], **Srikanta Basu**[1], **Khyati Bhatt**[1], **Amol S. Hosing**[1], **Renu Balyan**[2], **LalitBorde**[3], **Tapas K. Kundu**[4] **and Sorab N. Dalal**[1]

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Background: Promoting excessive genetic instability could be a potential target for anti-tumor therapeutics, as tumor cells are programmed to be genetically unstable due to the inactivation of checkpoint pathways and multipolar mitoses. Our work demonstrates that rather than inhibiting the activity of checkpoint protein Cdk1, a novel way of inhibiting tumor growth might be the premature activation of Cdk1 in interphase cells

Result: We have demonstrated that 14-3-3 family of proteins localize to centrosome and regulate centrosome duplication by inhibiting the function of G2/M specific phosphatase Cdc25C andCdk1/CyclinB1 complex that phosphorylates the T199 residue of centriolar linker protein NPM1. Loss of 14-3-3γ results in the hyper-phosphorylation of NPM1 at Thr-199, causing early centriole disjunction and centrosome hyper-duplication. Centrosome amplification led to aneuploidy and increased tumor formation in mice. We deciphered a way to increase the extent of spindle multi-polarity and thus reduction in clustering and pseudo-bipolarity by prematurely activating mitosis upon expression of a constitutively active 14-3-3-binding-defective-mutant ofcdc25C (S216A) in the 14-3-3γ knockdown cells.

Conclusion: Our findings uncover the molecular basis of regulation of centrosome duplication by 14-3-3 proteins and inhibition of tumor growth by premature activation of the mitotic program and the disruption of centrosome clustering.

B-29

Cobalt-containing Porous Organic Polymer (POP) as Precursor of New Electrode Catalyst for Oxygen Reduction Reaction

Yuping Yuan, Di-jia Liu

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A cobalt-containing porous organic polymer (POP) Co-PBY was prepared through trimerization reaction of the cobalt-bipyridine complex. In our cobalt doped polymer **Co-PBY**, high density of coordinated cobalt center has been incorporated evenly inside a porous network. Upon pyrolysis in an inert atmosphere, the porous organic polymer framework was converted into porous carbon support, converting the cobalt-bipyridine complexes into active species which showed good catalytic activity towards oxygen reduction reaction (ORR) in both acidic and alkaline electrolyte Such method of metal-doped POP pyrolysis provides an easy approach of achieving high density metal-nitrogen centers and potentially makes possible to obtain higher performance ORR catalyst. In this work, we will report the electrochemical, TEM, XPS, and surface properties characterization of the samples prepared from polymer **Co-PBY**. In addition, post chemical treatments on these samples produce an additional fine improvement of the catalytic activity that showed further possibility of application as non-precious metal catalysts for proton exchange membrane fuel cells.

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