BASIC ENERGY SCIENCES ADVISORY COMMITTEE
to the
U.S. DEPARTMENT OF ENERGY

PUBLIC MEETING MINUTES

JULY 29 – 30, 2014

Bethesda North Marriott Hotel and Conference Center
5701 Marinelli Road, North Bethesda, MD 20852

July 29 - 30, 2014
DOE BASIC ENERGY SCIENCES ADVISORY COMMITTEE
SUMMARY OF MEETING

The U.S. Department of Energy (DOE) Basic Energy Sciences Advisory Committee (BESAC) was convened on Tuesday, July 29, 2014, at the North Bethesda Marriot Hotel and Conference Center in North Bethesda, MD, by BESAC Chair John Hemminger. The meeting was open to the public and conducted in accordance with the requirements of the Federal Advisory Committee Act. Attendees can visit http://science.energy.gov to learn about BESAC.

Committee members present:

John Hemminger, Chair
Simon Bare
William Barletta
Gordon Brown
Yet-Ming Chiang
Beatriz Roldan Cuenya
Frank DiSalvo
Roger French
Bruce Gates
Ernie Hall
Sharon Hammes-Schiffer
Bruce Kay
Max Lagally
William McCurdy, Jr.
Monica Olvera de la Cruz
Mark Ratner
Anthony Rollett
Gary Rubloff
Maria Santore
Matthew Tirrell
John Tranquada

BESAC Designated Federal Officer:
Harriet Kung, DOE Associate Director of Science for Basic Energy Sciences

Committee Manager:
Katie Perine, DOE Basic Energy Sciences

Tuesday, July 29, 2014

WELCOME AND INTRODUCTION

The U.S. Department of Energy (DOE) Basic Energy Sciences Advisory Committee (BESAC) was convened at 8:35 a.m. EST on Tuesday, July 29, 2014, at the Bethesda North Marriott Hotel and Conference Center by BESAC Chair **Dr. John Hemminger**. Committee members introduced themselves. **Hemminger** reviewed the agenda and welcomed **Dr. Patricia Dehmer**, Acting Director, DOE Office of Science (SC).

NEWS FROM THE DOE OFFICE OF SCIENCE

In reviewing DOE and SC staffing, **Dehmer** shared that we are still waiting for the U.S. Senate to confirm political appointees to senior DOE positions.

The SC Fiscal Year (FY) 2015 request is $5,111M. The House marks are $5,066M and the Senate marks are $5,079M. The FY15 request for BES is $1,807M with a six percent difference between the House and Senate at 1,702M and $1,807M, respectively. Differences in the marks for SC will be adjudicated in conference. High Energy Physics (HEP) is the second largest SC program after BES based on an FY15 request of $744M. HEP will receive $30M more than the

President's request. The House and Senate support computing, and there is strong support for Nuclear Physics in part due to the implementation of their strategic plan.

Within the SC budget request, the Workforce Development for Teachers and Scientists (WDTS) Program saw an increase by the Senate of 51 percent. WDTS places undergraduate students at laboratories (labs), among other programs, and has been around for several decades.

There are philosophical differences between the House and Senate marks as well as their response to Federal Advisory Committee Act (FACA) reports for areas of SC.

The House report shows that BES' long-term success relies on balancing research, the completion of new facilities, and operating existing facilities. Both the House and Senate cautioned SC against assuming an ever-increasing budget. SC should balance it funding among facilities, construction, and research.

Dehmer pointed out the influence of FACA studies. The Leone Report, a study of novel coherent light sources in the late 1990s, led to worldwide interest after support for the Linac Coherent Light Source (LCLS) commissioning in 2009. Another example is BESAC's work on x-ray light sources to include an assessment of grand challenges. This led to a transformation of the hard x-ray free electron lasers landscape and enabled U.S. global leadership. FACA reports have led to significant facility funding and growth of the BES budget versus other parts of SC.

HEP funding in FY15 is low in anticipation of the HEP 10-year Strategic Plan (P5). The P5 has been accepted by the HEP Advisory Panel (HEPAP). The report proposes five scientific drivers and drove facilities funding recommendations. Appropriations staffers were briefed on the report. The House and Senate both increased the HEP FY15 budget by $30M over the Presidential request. This will help HEP become more robust.

The Fusion Energy Science Advisory Committee (FESAC) and Nuclear Science Advisory Committee (NSAC) are conducting studies. NSAC has garnered community support as well as House and Senate support for long-range plans.

Dehmer issued a charge to BESAC in February 2014 that includes examining the grand challenges. This is at a time when Congress is trying to hold the SC budget flat.

Dehmer shared a letter she sent in January 2014 announcing SC's continued commitment to funding new or renewal financial assistance awards of $1M or less in full. A copy of Dehmer's letter is available at http://science.energy.gov/~/media/grants/pdf/FullFundingMemo.pdf.

DOE is developing processes for digital data management with direction from the White House Office of Science and Technology Policy (OSTP) and the Office of Management and Budget (OMB). Laura Biven in SC is guiding the activity. As of 1 October 2014, all proposals to DOE must have a data management plan. DOE is the first agency to do this and SC is the first group in DOE to do this. The agency has produced a DOE Public Access Plan.

The Presidential Administration is continuing to consolidate all Federal STEM activities into three agencies. The FY14 President's Budget Request terminated several DOE programs to include the Computational Sciences Graduate Fellowship (CSGF). The Administration is expanding its discussion of STEM investments in 2015. DOE has mission-specific workforce needs in STEM fields and the DOE labs are a unique resource for training employees. Proposed STEM workforce development activities in SC will have to show an evidence-based statement of need, program goals, and a diverse applicant pool. All six SC FACA committees must show that there are unique needs that only the DOE can meet. Along with the labs, FACA committees have been asked to provide summaries that describe STEM needs.

The Senate added $10M to continue the CSGF and to broadcast the 2015 National Science Bowl Finals. Dehmer is pleased that WDTS has House and Senate attention.

Discussion

John Hemminger noted that some things in the 2007 Grand Challenge Report have yet to be implemented, but the report and stimulus money enabled things such as the Energy Frontier Research Centers (EFRCs). **Dehmer** added that Recovery Act funding of about $277M and a robust appropriation by Congress enabled EFRC creation. The timing of the report led to a large budget with the first annual EFRC appropriation in 2009 of about $100M.

Hemminger added that crystal synthesis and detector technology were two things that were not addressed. **Dehmer** suggested that the next report consider how to weave in recommendations from past reports.

Anthony Rollett shared that BESAC prioritized scientific facilities at DOE's request but he did not believe that this was reflected in the Senate and House comments about BES. **Dehmer** disagreed, noting that HEP, NP, and advanced computing are all competing for funds as there are many good ideas. Many good BES ideas were already funded and they are competing with ideas from other areas of SC. The SC budget needs to be expanded.

Hemminger believes that other SC offices have paid attention to ways that BES has achieved its success. **Dehmer** added that other programs and committees are delivering plans that are impressing Congress and OMB.

Hemminger suggested that BES address areas relevant to BES such as molecular-level environmental science that used to be supported by Biological and Environmental Research (BER). **Dehmer** noted that BER has not given up molecular-level environmental science. She informed **Bruce Gates** that the grand challenges direct thinking about science. The first five were solid and grand challenges should be big, like the HEP grand challenges. Sustainability was one of the first topics, and examples like this have caused researchers to think differently about their research.

Bill McCurdy commented that the report is only seven years old and wondered about the wording of the charge letter. **Dehmer** cautioned about putting too much weight on the words in the letter and that BESAC should not be restricted by the wording. **Harriet Kung** said that the intent of the letter is to give direction. The former charge was issued in May 2005. It would be good to re-think the challenges 10 years later. This may enable rethinking BES' portfolio and refresh how DOE looks at the most challenging scientific areas.

Dehmer noted that there have been stunning discoveries in HEP since the P5 report as they moved from science frontiers to five major scientific questions.

NEWS FROM THE OFFICE OF BASIC ENERGY SCIENCES

Dr. Harriet Kung, DOE Associate Director of Science for Basic Energy Sciences (BES), provided an update starting with the addition of new staff members. She also noted the passing of **Dr. Paul Maupin**, a BES Program Manager who supported the Catalysis Science Program.

The FY14 BES budget appropriation is $1,712M, an increase of $116M from FY13 but still $150M under the FY14 request. SC has been implementing full funding for financial assistance awards under $1M. The Division of Materials Science and Engineering (DMSE) and the Division of Chemical Sciences, Geosciences and Biosciences (CSGB) are exerting all options to maintain quality and success, and to reach overall portfolio balance across all BES programs. No-cost extensions for funding and other measures will result in a steady state after four to five years.

DMSE's renewal rate is down to 50 percent with CSGB at 40 percent in FY14. DMSE has larger grants and lab programs, while CSGB balances between labs and grants. New award rates for DMSE and CSGB are 15 and 20 percent, respectively. BES continues to integrate new ideas into its portfolio while keeping the integrity of vital areas.

FY14 saw many solicitations. The EFRCs are a successful example. Recovery Act funding ended dropping the annual budget by $55M and increasing the competition between the Centers. The new EFRCs are in 32 states and Washington D.C. Funding has been changed from five to four years to enable BES to open the EFRCs for additional solicitations every two years. Kung anticipates that there will be groups of solicitations and cohorts of similar sizes. Solicitations will be more frequent with the new schedule.

Thirty-two proposals were selected from about 200 proposals in FY14 and show an even topical distribution. The largest area with eight awards is Crosscutting Materials and Chemistry by Design at $24.8M. The awards involve as many as 14 other institutions to as few as two. Notable is the inclusion of DOE labs and universities within nearly all the Centers. Two awards include industry partners.

BES runs the Experimental Program to Stimulate Competitive Research (EPSCoR) awards appropriated at $10M. Three of 25 proposals were selected, and are being lead at Louisiana State University, the University of Wyoming, and Clemson University. The awards will start around August or September 2014. The Wyoming and Clemson awards include other DOE offices and programs.

The Ultrafast Materials and Chemical Sciences awards funded at $3.03M for FY14 will give nine awards starting around August or September. This will broaden BES' portfolio in anticipation of expanded capabilities at the Linac Coherent Light Source (LCLS and LCLS-II).

The Spallation Neutron Source (SNS) at Oak Ridge National Laboratory is operating at a record power of 1.4 MW and should continue at this level. Factors supporting growth from 1 MW since February include quality assurance improvements in target manufacturing and a new jet-flow design that mitigates target failure issues leading to longer target lifetimes. SNS awaits the completion of SNS Instruments Next Generation-II (SING-II) project. Four instruments will be built for neutron scattering and it is the last planned major item of equipment project for SNS. SNS currently has 17 user instruments with two more coming.

Construction on the National Synchrontron Light Source (NSLS-II) continues with CD-4 and approval to start operations around June 2015. Early completion is projected for September 2014 with the ring available to beamlines. The storage ring was commissioned, and the stored ~50mA beam was achieved in July 2014.

LCLS-II is revising the project scope based on BESAC guidance. SLAC and its partner labs have quickly ramped up to meet that guidance.

The Advanced Photon Source-Upgrade (APS-U) made similar revisions, providing upgrade capabilities in reaction to BESAC recommendations. It is nearing CD-1.

BES' FY15 request balances the research programs, facility needs, and community development of tools for BES research. Kung shared a list of initiatives in the FY15 request. They reflect tough choices and Administration priorities. BES will prioritize and use funds wisely.

The FY15 request is $1,806.5M. Computational Materials Science is a new activity, and construction and instrumentation are at desired levels. Other research programs are relatively flat. BES strives to balance research, facility operations, and construction/major item of equipment (MIE) projects.

BES sees a role for Federal stewardship in developing computational software and is pursuing this after several reports and after the Materials Genome Initiative was announced. The goal is open-source community code and software packages that include multiple length and time scales for discovery and prediction of materials functionality. Kung foresees up to four teams with multi-year awards for providing software as an explicit deliverable with an accompanying data piece. Current data shows that the top materials application running at the National Energy Research Scientific Computing Center (NERSC) is from Austria.

Computational Materials Science (CMS) will move from research use by experts to more general use by the community to speed the discovery and materials development. This is a tall order but the software piece needs to be filled. Open source software could reduce redundancies and allow core competiveness in the U.S. There are examples of early success such as the Materials Project at the Joint Center for Energy Storage Research.

The FY15 House mark for BES is $1,702M. The House fully supported research, provided $8M for CMS, and fully supported MIE, but was $10M under the request for the National Synchrotron Light Source-II (NSLS-II). The biggest impact is on facilities at $52M less than the request. Due to the language in the report, light sources and nanocenters would be reduced by about 10 percent from the request level. This would have severe impacts on staffing and users, and lead to intermittent shut downs. All facilities have been funded below their optimal levels for several years. BES is gathering impact statements for delivery to House staffers.

The Senate mark for FY15 reflects BES' request of $1,806.5M. Both the House and Senate have shown support for the EPSCoR program.

Congressional committees seem receptive to programs with clear strategic plans. The competition for funds is growing as others see how effective groups like BESAC can be to gain funding support.

Kung reviewed the BESAC Charge on Grand Challenges from 2005 that asked for the consideration of key scientific questions. An outcome was the report, "Directing Matter and Energy: Five Challenges for Science and the Imagination." Kung shared that it is evident that other countries review strategies like this and planning done by committees like BESAC when creating their own approaches.

The new charge is a chance to examine grand science challenges that BESAC previously provided and that have led to a transformational direction. It is a chance to shape the BES research portfolio for the next decade and century.

Discussion

McCurdy asked about the impact of a drop in materials sciences funding due to the full funding requirement, and its impact on universities in the BES portfolio, noting that funding overall is the same but being distributed differently. He asked if the numbers indicate changes over the coming years and if this is a steady state that will impact quality. **Kung** noted that renewal criteria are higher due to overall funding constraints. The move to a 50 percent renewal rate is a transition that will not end in three years but more like five. BES looks at the proposal quality and how it fits with the program's evolution. An analysis of the grand challenges with the DMSE and CSGB showed how the challenges influence the portfolio. One example are the number of proposals with "meso" in the title. Without a budget increase, pressure on the grant program will increase.

REPORT ON THE CENTER FOR APPLIED MATHEMATICS FOR ENERGY RESEARCH APPLICATIONS

Dr. James Sethian of Lawrence Berkeley National Laboratory (LBNL) and the University of California, Berkeley, described the Center for Applied Mathematics for Energy Research Applications (CAMERA). A diverse research team collaborates to build applied mathematics approaches to speed scientific discovery at DOE experimental facilities. The number of partners in CAMERA is growing beyond LBNL to the UC Berkeley campus.

Advanced mathematics seeks to provide things that users can use without becoming mathematicians and allow for building advanced mathematics in software applications.

Small investments can enable advanced science, decrease turnaround, and reduce facility costs, but require collaboration in close proximity at facilities. Mathematical boundaries are breaking down, and underlying mathematics and algorithms will ultimately be invisible or automatic to users yet allow them to push a button and get information.

The project began by solving programs for DOE's Advanced Scientific Computing Research (ASCR) program and capabilities being used in industry. These include understanding wind turbines, health and disease, the coal industry, inkjet printing, and industrial foams. Mathematics causes problems to be thought of in a different way.

CAMERA is looking broadly at SC facilities' mathematical needs. An important application is the use of computational tools for analysis, data reduction, and feature extraction *in situ*, using advanced algorithms and special-purpose hardware. Another application is post-processing to include reconstruction, inter-comparison, simulation and visualization. This is important since the math required is different than the math used for current and later challenges, and presents different questions. There are problems that have yet to be "mathematicised" and that require different types of math to meet challenges in a new climate for applied mathematics. These are represented by an explosion of work in new hybrid areas.

In big data, mathematics connects loads of data and computers. Data requires math to talk to computers, and math changes data into information. These challenges will get bigger with more data, complexity, noise, false signals, and unclear relational linking.

CAMERA is focused on computing structure from imaging, analyzing samples and proposed new materials, and designing new materials. There is a diverse range of occupations represented in CAMERA supported by a stream of young researchers interested in solving new challenges.

CAMERA delivers codes that run locally on computers at facilities, remote browsers that execute code running at facilities, codes that remotely run on data downloaded from facilities to supercomputers, and code that is downloaded and run remotely.

SHARP (Scalable Heterogeneous Adaptive Robust Ptychography) is a project that combines a high precision scanning microscope with high resolution diffraction measurements. The signal shows short-spatial Fourier frequency information. Phase retrieval comes from multiple diffraction patterns from the same region of an object.

In SHARP, math speeds things up by building a better starting guess. A software focus has led to open-source code. One application is intercalation battery research looking at mechanisms in lithium ion batteries. A goal is to give real-time feedback rather than the current one minute process time.

QuantCT is a project that provides automatic image analysis tools for micro-CT. Two-dimensional images are extracted and turned into 3-D and 4-D samples for quantitative analysis. At first, the project worried about filtering, but has moved onto segmenting near homogeneous regions and then microstructure analysis. QuantCT figured out how to take the Mumford-Shah function to simultaneously extract structure, then uses other methods to identify pathways. The technique is useful via software for microCT and detecting 3-D fibers.

PEXSI is a project that speeds electronic structure calculations for large-scale materials systems. The density functional theory results in a non-linear eigenvalue problem. A slow approach is to iterate, but PEXSI reduced the density functional theory cost calculation for general chemical and material systems.

A PEXSI breakthrough is representing the Fermi operator using a pole expansion. Selected inversion is used. Other topics include building discontinuous Galerkin basis functions and a new elliptic preconditioner. It is integrated in SIESTA, CP2K, and maybe in BigDFT and FHI-aims.

The Zeo++ project uses math and algorithms to design new advanced porous materials. Zeo++ allows for working with a number of chemical options and streamlining the process of finding things that are likely versus unlikely. An ultimate deliverable is a default tool for BES with a prototype interface for people to drive it.

The GISAXS and HipGISAXS projects look at x-ray scattering. Math is used to either compute a scattering pattern from a structure, or a structure from a scattering pattern.

Another project is reconstruction algorithms for X-ray nanocrystallography. This allows a macromolecule structure to be determined from a large ensemble of nanocrystals. There are algorithms that can solve problems such as the corruption of images with noise. Math can allow for using fewer images, more noise and harder cases. This can also address fluctuating scattering.

CAMERA is building, testing and exporting code.

CAMERA will need to find ways to continue to support ongoing software development for the DOE community and generate deliverables. The impacts include gains in productivity. With CAMERA, most users do not need to be mathematicians but can use tools that transform data into information that they want.

Roundtable Discussion

Hemminger asked how CAMERA could be replicated at other facilities, especially in ways that it uses LBNL and the university. **Sethian** believes that math's drawback and virtue is that it is portable. It is important for groups and students to go places, and CAMERA can work with mathematicians at other places. Just one-tenth of a $500M annual operations budget could make a real dent.

Rollett asked if this could be applied to computing tomography with diffraction experiments as applied math is often missing from this type of problem. **Sethian** shared that CAMERA was initially focused on things that other groups at the lab were doing, but has reached to others. Communication challenges occur when CAMERA gives an unexpected answer.

Max Lagally noted that CAMERA addresses properties examples that are not necessarily materials discovery problems or mesoscale phenomena. **Sethian** noted that CAMERA's problems selection was based on funding. The math community needs to bring its computational techniques into experimental measurements and try to get them closer. In the mesoscale area, the challenge is having small to talk to large.

McCurdy commented that in working with murky data there is often an impedance mismatch. He asked if math formulas might present a different view when applied to murky data. **Sethian** agreed that murky data is a rich area for math. He noted that those in math and physics tend to accept solutions even when others are convinced of the answer. CAMERA links these people. Mathematicians can collect enough data near the target positioned by engineers to generate conclusions, and use new techniques to help traditional fields. There is an attempt to rule out impedance mismatches and ask partners to promise that what they want is really what they want. Others in the same field have the problem they are addressing is the right problem.

Frank DiSalvo asked if the underlying math should be invisible to users. Materials scientists may not know if questions they are asking are beyond the range of the tools being used. Hence, they do not know if any errors are systematic. Users could fall into believing what they are receiving. **Sethian** noted CAMERA makes students write code from scratch. He also thinks that some content can be packaged to give a hint of doing them automatically. There should a continuum from manual to automatic. CAMERA needs to work with different types of users to make this useful and credible.

PRESENTATION OF THE JCESR UPDATE

Dr. **George Crabtree** of Argonne National Laboratory provided an update on the Joint Center for Energy Storage Research (JCESR) Hub. The Center is 1.5 years old and thinks about energy storage very differently. It is proposing a new paradigm for doing battery R&D due to huge opportunities for new approaches in this space.

Transportation and electricity are two big energy uses poised for transformational change. The bottleneck for transitioning to greater electricity use for transportation and moving to an electrical grid based on renewables is inexpensive, high performance electrical energy storage.

JCESR wants to deliver electrical energy storage with five times the energy density and one-fifth of the cost of today's commercial batteries within five years. The Hub aims to have legacies that include building a fundamental science library that show successes and failures, building car and grid battery prototypes, and a battery R&D paradigm that integrates discovery science, battery design, prototyping, and manufacturing collaboration.

JCESR's aggressive approach seeks to be transformative, to meet the need for next generation energy storage for next generation energy technologies, and to bring the community's attention to the potential beyond lithium-ion. Lithium ion technology increases energy density and decreases in cost per year but cannot yield required transformative changes.

JCESR proposes to apply genomic ideas to liquid organic materials or electrolytes. Computing helps find the 10,000 candidate materials and the 10 that could be good materials for batteries. The Electrochemical Discovery Lab allows for synthesizing and characterizing with wet and dry electrochemical interfaces. The paradigm uses techno-economic modeling to build battery systems on the computer. JCESR then looks at technological and manufacturing costs. JCESR uses a four component set up for prototyping to recognize where problems exist and to direct problems to one of four teams.

JCESR takes the traditional lithium ion battery rocking chair model and applies to it a mutivalent intercalation system to double or triple capacity stored and released. To do this, JECSR must find battery components that will work together. Another approach focuses on chemical transformation, replacing intercalation with high-energy chemical reactions. JCESR is also trying to replace solid electrodes with liquid solutions or suspensions to achieve lower costs, higher capacity, and greater flexibility.

Lithium-ion has been at a commercial level for 20 years but can get better. The space for transformational advances is huge. A combination of new systems and around 20 to 30 different materials could be implemented in these systems, achieving 100 different ways to build new types of batteries. JCESR does not start with a battery that it thinks it will end up with but starts with concepts and tests them.

JCESR has gathered 65 cross-sector affiliates that are supporting parallel research across four functions and using frequent communication to inform strategic directions. It has also defined the prototype that it wants to make based on an advisory committee review in October 2013. Battery technology readiness levels are informing the progress that JCESR needs to make over the next five to 10 years to achieve scale-up of new materials, cell testing, and transfer to a commercial partner to enable the scale-up to transfer and production.

One highlight of JCESR's work is recognizing that trace water catalyzes lithium peroxide electrochemistry. Water affects the outcome of this reaction and could impact every type of battery as well as other areas of electrochemistry. Another discovery is recognizing that a gaseous electrode can help to assemble a lithium-air battery but that a purification system must be built in that adds weight. This reduces the appeal of liquid oxygen. JCESR has also learned that quinoxaline can enable production of an all organic redox flow battery that can provide 10 times the electrochemical activity.

The problems to be tackled by JCESR are many for a multivalent intercalation battery and include the mobility of ions in cathode, solvation and desolvation, and electrolyte stability. JCESR has also been able to make a full cell that has an anode, electrolyte and cathode that all appear to be compatible. JCESR has built the first magnesium ion battery in 14 years.

Future work includes looking at metal anodes, the solvation cell and cataloging all solvation cells of working electrolytes, understanding Li-polysulfide semi-flow, and prototyping the outcome of this work. Work includes finding novel prototyping concepts to achieve a gravity induced flow cell, and learning more about the interactions between lithium and sulfur and how they can interact with electrolytes.

Roundtable Discussion

DiSalvo commented that JCESR's work is incredibly ambitious. **Rubloff** asked about work on the grid. **Crabtree** shared the JCESR's all organic redox flow is a candidate as is the lithium poly-sulfide flow battery. The batteries must be cheap, recyclable, and made big. Grid options are more diverse with many applications. For instance, control could be shifted by milliseconds to save energy, or a wind farm could be backed up at night to store energy for day use. JCESR hopes the grid community will seek help with specific goals from among 15 or 20 applications.

Hemminger noted that PCB transformers embody the positive qualities of organics but expressed some concern. **Crabtree** thinks it is too early to see if this prototype will be the commercial battery. Specific compounds have yet to be considered. Safety issues can be thought of during design, along with decisions about derivatives and breaking things down to parts that are not helpful.

Lagally noted that grid storage once brought up talk about superconductive energy storage the size of football fields, and asked if JCESR has thought about that. **Crabtree** shared that this is one way to store energy, realizing that there is a window in the storage arena for achieving something.

Rollett pointed out that scaling can lead to bigger systems that react in unanticipated ways and produce undesirable reactions. **Crabtree** agreed that scaling up reveals unintended consequences hence JCESR conducts computer-based simulations such as those involving Li-sulfur to understand the possible reactions before moving to a prototype stage.

PRESENTATION OF THE BIG IDEAS SUMMIT AND DOE TECH TEAMS SUMMARY

Dr. Steve Binkley, Associate Director, DOE Advanced Scientific Computing Research, shared findings from the Big Ideas Summit and the work of the DOE Tech Teams.

The Tech Teams have been identified as Secretarial priorities and reach across DOE to collaboratively focus DOE skills on these topics.

The Advanced Computing Tech Team is creating a network of Advanced Computing for Energy – Innovation Capabilities (ACE-ICs) to bring petascale computing to energy technologies. Useful and usable computational capabilities to address challenges in areas such as wind farming are emerging. SC's role is to make the Sci-DAC for Energy approach used in SC, to share multi-scale methods for chemical and materials systems, to provide a connection to ESnet, and to document requirements for programs.

The Clean Energy Manufacturing Tech Team develops and maximizes the application of advanced technologies to push manufacturing toward energy goals, and to strengthen U.S. manufacturing competitiveness. An outcome is the creation of Clean Energy Materials Manufacturing Centers of Excellence. The first pilot Center will be stood up in 2016.

Grid modernization is another focus. The U.S. has three interconnected grids that need to be re-configured to support improved energy consumption and better energy use. This must be done while remaining resilient to multi-faceted challenges. The Grid Modernization Tech Team uses institutional support and industry partnerships to achieve integrated system testing.

The Supercritical CO2 Tech Team is working toward movement from a Rankine Cycle to a Brayton Cycle to ultimately shrink the size of a turbine from 20 meters to about 1 meter while maintaining an energy output of about 300 MWe. This technology could be applied in areas such as solar central power cycles, nuclear energy, and space solar electric propulsion. It is hard to find materials that hold up to the temperature and pressure of supercritical CO2.

The Subsurface Technology and Engineering RD&D Tech Team looks at knowledge of the subsurface and its role in understanding how it can support energy storage, handling energy waste, and supporting energy needs. The team is examining how to use data gathered from drilling operations and other applications. A workshop in March 2014 identified multiple challenges for the Team's consideration.

The Water Energy Tech Team looks at the water-energy nexus. They have used the LLNL model that shows the spectrum of sources of energy and where resources end up being used, and added in water consumption related to energy use. The Team is exploring the intersection of energy and water use to find ways to reduce water use. Data, modeling and analysis are one component of their work. The team will explore technology RD&D to identify technologies that can be optimized for reduced water use and related policies.

Binkley summarized the Big Ideas Summit held in March 2014. The Summit focused on reinforcing the DOE National Laboratories' role as strategic partners with the DOE to catalyze collaboration. The labs provided the DOE with eight topics to be considered at the Summit. Many topics have been incorporated into the work of the DOE Tech Teams.

Roundtable Discussion

Rollett asked how much of advanced computing ended up in the lab big ideas summit. **Binkley** shared that simulation and advanced simulation was addressed at the Summit since every idea included advanced simulation. Similarly, the Tech Teams focus on simulation activities as some teams cannot do real world testing and collect data through simulations instead.

Ernie Hall commented that wind farm plant performance was mentioned and wondered if the Office of Energy Efficiency and Renewable Energy (EERE) had a sense of how to engage those who build wind plants. **Binkley** noted that there are those in DOE and labs who know how best to engage the wind farm industry. Of interest are the computational needs to be applied to a specific class of industry problems. Calculations may be run on supercomputers since the industry uses desktop machines. Shaping code for that industry and getting codes hardened can be difficult. Research codes are part of the challenge.

Hemminger mentioned the grid and reliability, citing that the grid is more reliable in Europe and Japan. **Binkley** shared that part of the problem with the average down time is that it comprises many data points from the grid. Europe and Japan differ as an outage may occur in the suburbs for 10 days whereas other areas may not have an outage. Some countries have better designed architecture designed from the ground up for reliability. Infrastructure replacement is a challenge that the Federal government can help inform as it will have to happen in the coming decades.

PRESENTATION ON THE CHEMICAL SCIENCES, GEOSCIENCES, AND BIOSCIENCES (CSGB) COMMITTEE OF VISITORS (COV) REPORT

Dr. Sharon Hammes-Schiffer informed BESAC that the CSGB COV was conducted from April 30 – May 2, 2014, and looked at the efficacy and quality of processes used to manage proposals, projects and programs. It examined the breadth, depth of portfolio elements, and CSGB's national and international standing of those portfolio elements.

The COV consisted of three panels and 17 members, some of whom had prior COV experience and were funded by BES. The COV used preliminary information and conference calls, and then met with program managers to review the programs. This was followed by the readings of folders, and the finalization of findings and recommendations.

The COV found that proposal solicitation, review, documentation and monitoring are outstanding, with a comprehensive and thoughtful review process. The breadth and depth of the portfolio elements and quality of the science and principal investigators (PIs) is excellent. Program Managers (PMs) successfully balance the mission of the DOE with the flexibility to produce high-quality scientific research. It was recommended that program managers be able to travel to national and international meetings, and visit the labs of researchers in their programs.

The receipt of white papers as preliminary statements of potential research projects is favored by PMs as it permits help and rapid communication with a potential PI. The COV recommended the continuation of this practice.

The COV was pleased that Portfolio Analysis and Management System (PAMS) has started although it is not yet fully implemented. The COV recommended that implementation be finalized as soon as possible to support data analysis.

BES should implement a strategic planning session at the division level to evaluate current directions and to identify new options and synergies. This will allow for communication and collaboration in BES and develop PMs' respective portfolios in a consistent, cooperative manner. Planning should be ongoing at team and division levels, and use internal and external sources.

Additional suggestions include providing mail reviewers with clear instructions about the review criteria and ensuring some greater familiarity with national labs.

The funding balance between proposals with single PIs and those with multiple PIs is of community interest yet quantifying the levels of productivity that come out of one type or another is challenging. Metrics would help DOE balance this and enable it to be maintained and discussed in the community.

The use of white papers has led to higher apparent acceptance rates as some pre-proposals are halted. PMs should keep track of white papers, which proposals had white papers and which did not, and which ones were stopped before being submitted.

The COV encouraged further documentation of cross-program collaboration and interaction.

Compared to the COV held in 2011, three of the four recommendations for the 2014 report were in the 2011 report and have been addressed in some way. BES concurred with the three recommendations and agreed to implement them within fiscal constraints. The recommendation to hold a strategic planning session at the division level is new and could help transmit the overall vision from the core program to empower the division and programs while overcoming individual views of priorities.

Roundtable Discussion

William Barletta noted that striking balance is a hard problem and wondered if that can be connected with tracking responses to proposal white papers. The goal is to keep people from doing excessive work on a proposal that may not be accepted. He asked if the COV discussed how to share metrics earlier with people writing papers and if there is a template to guide paper development. **Hammes-Schiffer** sees paper tracking as difficult due to the many forms and how differently the PMs track the interactions. The overall practice can save people time. She cited the 200 proposals in the EFRC and possibility that 2,000 people were involved to some extent. The white paper approach could identify how to lessen the time spent on non-suitable proposals. **Kung** shared that BES takes COV input and the burden of the proposal preparation seriously. Future EFRC solicitations are expected to be targeted. BES will form a plan for this with the idea that a white paper be considered along with limiting the scope of topics. **Hammes-Schiffer** suggested that this could decrease authors and reviewers' workloads.

Hemminger asked if there is a way to generate input from the community and PIs on the new recommended strategic planning process. **Hammes-Schiffer** noted that this could be tied to the grand challenges charge. PI input could come from their involvement in meetings in which they are already involved and PMs could engage them at that time. The COV did not propose extra workshops but rather informal ways to discuss hot topics in the field.

Hammes-Schiffer responded to **Bruce Gates** that the COV did not benefit from PAMS as everything for this review was in hard copy and in individual folders.

Hammes-Schiffer shared with **Gates** that the COV team size seemed right. All were able to give input and represented expertise in multiple areas. The breadth of expertise may depend on the structure of the BES.

Yet-Ming Chiang wondered if there is a timeline for funding hot emerging areas, and if it seems like too many people jump onto emerging topics. **Hammes-Schiffer** shared that PMs are always looking for new areas. PAMS might show the quantitative data Chiang is looking for. PMs and PIs talk constantly and form impressions of topics based on white paper submissions. PMs can keep the right balance and phase topics in as appropriate.

Hammes-Schiffer responded to **Lagally's** question about expanding the timespan between COVs. Even if the same issues are coming up they should be restated. The need for PAMS implementation is an example. **Kung** added that the three-year cycle is unlikely to change and provides a good timeline for seeing portfolios' progress. It also assesses the efficacy and standing of a program, and where it needs to be. Support for travel needs to be reemphasized.

The funding for this is the same one that pays the salaries of program staff and PMs, and Congress continues its efforts to shrink this pot of money.

Gordon Brown chaired a COV in 2005. He is disappointed that progress on travel funding has not been made in nine years. This would permit better evaluation and conference attendance. **Kung** argued that more funds for staff and travel have been added but that it stopped due to overall holds on travel for all agencies. This is a constant point of attention for BES.

BESAC voted to accept the COV report and it was unanimously approved. It will be sent to the SC Director with a response from BES.

UPDATE ON THE WORKFORCE DEVELOPMENT NEEDS IN SC RESEARCH DISCPLINES CHARGE

John Hemminger and **Pat Dehmer** presented a charge at the February 2014 meeting wherein Dehmer asked for data on BES-relevant disciplines not well-represented in U.S. academic curricula, and disciplines in high demand both nationally and/ or internationally resulting in difficulties in recruitment and retention at U.S. universities and at the DOE national laboratories.

Hemminger gathered input and summarized the input for Dehmer. SC welcomes additional input from BESAC. Hemminger reviewed the comments for the BESAC which included:

- There is a tremendous amount of applied electrochemistry being done in U.S. institutions and national labs, but fundamental electrochemistry is rapidly disappearing from U.S. curriculum. The average age of senior electrochemistry faculty at U.S. universities is higher than in Europe and other countries.
- Nuclear and radiochemistry, to include actinide and lanthanide science, are areas in which U.S. academics is weak
- Chapter seven of the BESAC 2007 Grand Challenges notes that crystal growth is an area that needs attention
- Computational sciences needs focus as it is becoming more important to BES' mission
- Most fundamentally, new instrumentation is not being invented in the U.S. It would be useful to determine the number of beam-line scientists at BES facilities earned a PhD in the U.S.
- Detector science and accelerator science both need attention

Roundtable discussion

Beatriz Roldan Cuenya noted U.S scientists do more applied work while those in Europe do more work with theorists and in fundamental ways. She believes that BESAC needs an industry viewpoint, too. **Cuenya** also noted that most instrumentation is required immediately forcing a trend to wait for something to be built. In Europe, research grants are for five years. In the U.S., we report annually.

Rollett commented that the U.S. technologist training is not as good as that for scientists.

Hemminger told **DiSalvo** that BES' process started when other FACAs were developing strategic plans and that these responses were folded into their strategic planning process. **Hemminger** sees that BES will have the opportunity to explore these questions in the next BESAC charge.

PRESENTATION OF THE GRAND CHALLENGE UPDATE AND INITIAL DISCUSSION OF THE BESAC CHARGE

Mark Ratner, George Crabtree, Graham Fleming, and **John Sarrao** agreed to be on the executive committee and will lead this follow-up discussion. Nearly all BESAC members have agreed to join in the discussion over the next few days. Some will join the working group that will write the report.

Hemminger explained that in 2007 there was an initial BESAC meeting with smaller working meetings at different places in U.S. The grand challenges evolved into a set of questions. The current process will be the same but requires additional work to include three meetings over the next six months in different places. The 2007 report has had a huge impact and influence on the international research community.

Ratner described the process used to produce the 2007 Grand Challenges Report. A set of challenges defined BES' discovery science portfolio. This drew on a number of published reports from the four years prior that should still be considered. The topics were not necessarily striking but included things like the mastery of matter, and complex and emergent phenomena. In 2006, criteria for a Grand Challenge was defined and used to winnow down scientific areas. This resulted in five new topics representing interconnected themes. The title of the report was "Directing Matter and Energy: Five Challenges for Science and the Imagination."

The process pointed out many things that are still unknown. Theory, as an example, was still in its infancy. It also led consideration of needed technologies, facilities and infrastructure, education and training programs, and things such as a DOE Energy Institute. Many considerations did not evolve and many scientific questions were not answered.

Some aspects of the report worked well and excited people. For instance, the EFRCs were started. There were scientific achievements, to include thinking about nano, understanding and control of chemistry at the single-bond level, and plasmon-enhanced subwavelength lasers. The 2007 report did not consider data science. The current committee is forced to think about what is important now.

Sarrao talked about how meso has emerged since the last grand challenges report. Mesoscale science presents challenges that can move beyond nano and into the continuum. There is a clear sense that there is an open space in the middle, from the quantum to the continuum. This is a ripe space that flavors the grand challenge discussion by looking at understanding of reductionism and how it has fed into constructionism, and how that can inform knowledge at the atomic scale. There are six priority research directions that have emerged from mesoscale science, the alignment of which may appear through the grand challenge questions.

The implementation mechanisms that can advance mesoscale science need consideration. It is not merely looking at the grand challenge and what needs to be done, but how to get there.

To develop the mesoscale report, the broader community gave broad input that guided how the mesoscale report played out. This action should encourage the Grand Challenge Report authors to cast the net broadly and get input to help shape their thinking.

Crabtree asked BESAC to look at specific questions. The charge requests evaluation of "the breakthrough potential of current and prospective energy science frontiers based on how well the research advances the five grand science challenges." The report will advise BES' development of research strategies for sustained U.S. science innovation and energy research leadership.

The subcommittee will need to think about the report title, how to assess current challenges and consider new ones, answer whether or not the prior challenges really made a difference, and how to build on past success.

The website for the effort is www.besac-grand-challenge2014.com. It includes the agenda for upcoming subcommittee discussions, and will host presentations given at meetings.

Roundtable discussion

Hemminger requested input from everybody and not just BESAC members. Inputs can be presented via quad charts available on the Grand Challenge website.

Matthew Tirrell noted that the report should include less grand actions that can support big results, to include needing more beam line scientists. Everything that is needed should be described in an exciting way.

Hemminger responded that a plan is laid out for subcommittee discussions.

Gates noted the need to do this again in seven years.

DiSalvo noted that the stage for what will come must be set and communicated. The report sets the stage for unanticipated discoveries.

Rubloff asked how to know if the effort has succeeded and how progress can be measured.

Hemminger responded that previous grand challenges were seen as 20 and 50 year issues and great science has been done during the past eight years. BESAC should focus on identifying the grand drivers in the community. The questions that are posed will be substantive challenges.

Lagally added that proposal submissions are an indication that people are responding to the grand challenges. He suggested that the challenge now is to avoid just adding sub-bullets to the last grand challenges.

French urged that BESAC be prescient, set direction and highlight challenges, but also be open to external things that will impact work in the community.

Tirrell noted that the term grand challenges can be misconstrued as grand promises. Using mesoscale as an example, the community might not know how to solve every challenge but knows that it has a basis for solutions.

Barletta shared that things like instrumentation should be written up to show the need for capabilities and facilities. An example is the need for optical technologies at all different scales. To be leaders and make challenges doable, critical enabling things are needed. **Rollett** agreed, suggesting a focus on energy frontiers.

PUBLIC COMMENT

None

Day one of the BESAC meeting was adjourned by **Hemminger** at 4:50 p.m.

Wednesday, July 30, 2014

PRESENTATION OF THE EVOLUTION OF THE ENERGY LANDSCAPE

Dr. Ellen Williams, Senior Advisor, Office of the Secretary of Energy, DOE, told BESAC that the world has increased in complexity as it moves to more convenient, accessible sources of energy. New technologies start out small and seem clunky but can have dramatic impacts over time. Oil well technology is an example. Technology can be safer, cleaner and more efficient over time.

There have been transitions in how we get energy, moving from wood to coal oil. Still, the amount of biofuels being used now is the same as it was 100 years ago despite using more of all forms of energy. An increase in the concentration of CO2 in the atmosphere is one outcome. In 1960, the atmospheric CO2 concentration was 320 ppm and we have since passed 400 ppm. The increase is having an extreme effect on ecosystems and how the world functions. Scientists believe that this must be held to 450 ppm for no more than 2°C in global warming.

The energy system is very big, making it hard to keep everything in context. To understand overall consumption, the world uses the equivalent of 16,000 gigawatt power plants per year or 12 billion tons of oil per year. There are differences in fuels and how they affect the future. Fuels with more hydrogen tend to have higher energy content and lower CO_2 content.

When Williams started her research, she thought that water would have an important role in energy but learned how energy is more connected to our atmosphere in terms of CO_2. About 10-15% of water use is for the energy sector. Most water use is tied to agriculture.

We can map energy sources to conversion devices to show that energy is not used frivolously but is used for what we want. Oil is primarily used in diesel engines then cars, trucks and planes, and then needed for passenger and freight transport. This all impacts structures, sustenance, food preparation, hygiene, thermal comfort, communication and light. Thermal comfort is one of the biggest energy uses and one that can improve.

CO_2 emissions research shows that oil, natural gas, and coal amount to about 60 percent of all greenhouse gas emissions. The other 40 percent are things such as fluorocarbons, N_2O, and methane from biological processes, agriculture, and waste management.

The DOE and other agencies do regular energy projections but they do not demonstrate what should happen but what is likely to happen based on what we know now. Energy use should level off in the developed world but will grow in developing nations between now and 2035. Energy use will increase by 30 percent over the next 20 years, mostly from increases in oil, and a faster increase in gas than projected few years ago.

The International Energy Agency (IEA) projects that CO_2 production will increase dramatically and that we will reach 800 ppm by 2100 in a business as usual scenario. Even if we hold emissions constant, we are looking at 600 ppm by the end of the century. Unfortunately, CO_2 stays in the atmosphere for hundreds of years. A 50 percent increase in CO_2 production by 2099 could produce about a four degree Celsius increase. This means that consumption must decrease. Energy use should be cut and oil use should lessen.

Looking at gas, the combined cycle gas turbine is very efficient. When adding a CO_2 tax of $40 per tonne, the price goes up by about 10 to 15 percent. If carbon capture and storage are added, then the price might double. Still, carbon capture is still an expensive way to reduce emissions.

Looking at coal, much of it is used to produce electricity and coal plants have long since been paid off. If a carbon tax is added to this, the cost would become higher than the present cost of electricity and even higher with carbon capture and storage.

Looking at low-carbon sources, geothermal is very price competitive and can be run year round along with nuclear and bioenergy production. Wind is attractive but very competitive. Solar photovoltaics is likely to come down in cost, and concentrating solar power is still very expensive but may come down. When doing a cost comparison, the simple cycle gas turbine is in about the middle of all other technologies.

Williams discussed reserves and resources for energy sources. The U.S. thought at one time that it might run out of oil. That is certain to not happen for coal. Energy resource research has found sources that are too expensive to produce, others that need exploration, and some that we know we can produce. This last group is the reserves.

One reserve is copper. In the 1970s, global reserves were 280m tonnes. It was believed that the copper reserve to production ratio will last about 40 more years. Since the 1960s, production exceeded the estimated availability and the reserves rose to 630m tonnes. The reserve figures grew significantly.

Oil projections indicate that there is about 1,000B barrels of oil in the Middle East and we have produced 1,000B. Oil is also produced in Canada and Venezuela for about $100 per barrel. Natural gas and coal can also be used to produce liquids. Biofuels are also a competitive alternative to oil due to the high cost of oil.

About half of all production between 2020 and 2035 will be traditional oil and gas. The other half will be unconventional oil, shale gas, and renewables. The latter will increase to meet increasing global demand.

The U.S. is a lead producer of shale gas in the world and will become more so as most of the world's production will occur in the U.S. Exporting shale gas will be a slow process due to technology transition in other places.

The DOE and IEA project that future consumption in the U.S. will be flat, with decreased or a flattening consumption of oil and coal. Renewables use is projected to grow from 8 to 10 percent by 2040 with increases in natural gas production. More oil and gas use would lead to higher CO_2 emissions. However, proposed regulations such as GHG10, which would add $10 per tonne CO_2 then increase that cost by five percent per year, and GHG25 would dramatically lessen emissions.

Technology has a huge role to play, especially when it is balanced with different regulations. Technology projects are looking at reducing CO_2 releases with more renewable generation, nuclear energy production, biofuels, increasing electrical vehicle use, and changes in industry.

Those giving projections need to take a systems perspective to understand what needs to be done. Solar fuel is an early stage technology example, wherein CO_2 is taken out of the atmosphere, processed, and used as solar energy. Agriculture is fairly inefficient in how it uses sunlight but photovoltaics could give higher capture and make an impact in biofuels. Another example is looking at hydrogen production and ways to improve hydrolosis to produce hydrogen.

The cost scale for technologies depends on operation expenses. Bigger plants have lower operating expenses per unit of energy. Researchers compared a large nuclear source with a fairly large solar plant and found that the facility was smaller and running less efficiently. Hence the investment made in capital equipment was not useful. The best way to make comparisons is to look at how renewables would fit into overall electrical systems. Those comparing different costs of sources have to be careful as there is a need to view combinations of different sources.

Williams urged care in how science is communicated.

Improvements are needed in existing technologies, and there is room for new discoveries and how we approach understanding new systems. Scientists cannot be naïve about the context in which they work as economic and policy costs drive decisions that are made in that context.

The value of fundamental research should be better understood and has an economic value.

Roundtable discussion

Rollett asked where fundamental research has paid off. **Williams** noted that DOE's investment in wind, as an example, may have a return on investment of 3:1. Multiple views are required when identifying payoffs, and care is needed when sharing results as there can be a lot of skepticism.

Chiang asked why the U.S. will be a shale gas leader. **Williams** pointed out that the U.S. has shale gas formations in relatively flat areas so the strata are parallel. Large deposits of shale are more easily hit. Shale is very diverse and it took about 20 years to find which formations and processes would work. The U.S. also has a large oil and gas production infrastructure, and that can drive research and development quickly. This has to be built up in other countries and has large upfront costs meaning that they are less likely to do that.

McCurdy asked why U.S. consumption and CO2 energy-related emissions seem to level out around 2015, and what would cause demand to be so elastic that predictions of the impact of a CO2 tax would be dramatic. **Williams** explained that greater efficiency in the transportation sector is reasonable for leveling out. Also, most companies believe that we will not see dramatic increases for fuel in U.S. One big factor is a vast improvement in the amount of energy use per GDP in the developed world.

McCurdy asked about demand elasticity as a driver of the dramatic decrease. **Williams** believes that this is due to the cost of electricity, decommissioning of local plants, and the sudden switch from coal to gas but she would have to confer with other DOE colleagues. There are other efficient resources and technologies that will also kick in around 2015.

Williams shared that from a global perspective, the world economy as a whole has more powerful responses as the U.S. has a more mature infrastructure but one that takes longer to change. Williams offered the guess that it takes the rest of the world longer to build their infrastructure and they are at a stage where they can make changes.

Barletta noted a chart with carbon and methane on the bottom in terms of CO2 equivalents, and wondered if trends in global population growth will offset energy efficiency gains. **Williams** noted that the biggest concern is land use change and deforestation. Intensified pasture use and more methane due to livestock could be big problems.

Gates asked about energy production, consumption and transportation issues. **Williams** shared that transportation is an issue especially with natural gas. For a long time, natural gas costs followed oil costs, but that changed as natural gas is less fungible than oil. It is still relatively easy to change the price of oil and transportation costs. Natural gas is still harder to work with. These comparisons require looking at a balancing of prices. China and Japan are paying four times as much for natural gas as they lack decent transportation infrastructure.

Williams shared with **Brown** that nuclear energy could have a huge impact. Nuclear energy resources globally have been insufficiently stewarded, and nuclear waste has not been handled efficiently. Underground storage is viable but takes a lot of effort. Nuclear issues can be solved but the U.S. has not done this well in the past 50 years and has to do a lot to convince people. China is building nuclear energy capabilities at an amazing rate and all can hope that that is successful. How China will manage nuclear waste disposal is an interesting question.

Hemminger asked about the accuracy of shale gas reserves in the U.S. **Williams** noted that estimates vary and people need to estimate based on reserves. She is aware that shale resources in California are more expensive to produce than in other places.

Rollett noted that people often talk about installing their own energy efficient systems. **Williams** commented that people address in this in a systematic way but the number who do things such as driving electric vehicles is very low, and those with the economic resources to make efficient choices is small. Projections of energy efficiency do account for human behavior.

SUMMARY OF THE FUTURE OF ELECTRON SCATTERING AND DIFFRACTION WORKSHOP

Dr. Yimei Zhu told BESAC that the Future of Electron Scattering and Diffraction (FEWD) Workshop held in February 2014 looked at opportunities in electron scattering and diffraction that can inform the BES grand challenges. The workshop looked at scientific frontiers that require advances in electron scattering and diffraction and the new science that could be created.

BES sponsored the TEAM project that enabled advanced imaging and resolution. The scientific case for improving resolution alone is not sufficiently compelling, yet there is scientific motivation for better molecular/atomic resolution measurements of functionality at short time scales and in real environments.

There are four science areas that can be impacted by electron scattering and diffraction advances: multi-dimensional visualization of real materials; atomic scale molecular processes; photonic control of emergence in quantum materials; and, evolving interfaces nucleation and mass transport. There are three instruments that can enable advances in these areas.

Zhu described the challenge inherent in the area of multi-dimensional visualization of real material. For example, thermoelectric energy harvesting requires the design of materials with low phononic heat transport and high electronic conductivity.

Work in atomic scale molecular processes seeks to understand and control the selectivity and efficiency of photon energy conversion.

Research in the photonic control of emergence in quantum materials is focused on disentangling and controlling competing lattice, charge, spin and orbital order. Future instruments will have tailored intense electric field pulses and tunable multi-cycle optical excitation, as well as the use of ultrafast electron probes to disentangle locally competing order parameters.

Evolving interfaces, nucleation and mass transport research is challenged by the imaging of interface dynamics, mass transport and nucleation events at molecular and atomic levels.

Instrumentation needs include a multidimensional atomic resolution electron microscope that will allow accessing structural information over real, momentum and energy space at low temperatures. A future microscope would have advanced spatial resolution, better transmittance, and greater stage stability.

An ultrafast electron diffraction and microscopy instrument is another need that would permit imaging and controlling materials processes in real-time and real-space. This instrument would be complementary to the x-ray free electron laser (XFEL). This equipment would improve time resolution over current microscopes by at least 1,000 times.

A 'lab in gap' dynamic microscope would permit the quantitative measurement of materials in structure, composition, and bonding evolution in a working environment. Currently, the highest resolution has a five mm gap at 0.5 Å. The goal with a new microscope would be a 10 mm gap at 1 Å.

Some key developments are required for the 'lab in gap' microscope such as differential pumping; correcting for spherical and chromatic aberrations; and the synergistic development of optics, source, sample environment and detectors.

The FEWD Workshop pointed out that BES should aggressively support R&D of complementary and enabling instruments to advance physics, chemistry, materials science, engineering and technology, and other fields.

Roundtable discussion

Zhu shared with **Gates** that the U.S. has had direct involvement in instrument development especially in places like Chicago. For ultrafast, there are some labs that are working on high energy ultrafast instruments. Florida State University and Michigan State University are looking at low energy ultrafast equipment. It is hard to compete with Europeans manufacturers as there are early-career developers with the capabilities to modify this equipment.

Rollett asked about proposed dynamic measurements when there is actually dynamic TEM with already apparent similar characteristics. **Zhu** suggested that ultrafast electron diffraction and microscopy is an area that requires looking at specifications that are different and propels the need to achieve more in this area. Current resolution levels make it hard to understand chemical processes.

Rollett asked if tomography would be a useful area of the work that Zhu described. **Zhu** confirmed that three-dimensional tomography has been demonstrated. The challenge is whether or not it is possible to measure the potential electromagnetic field in 3D. There are a lot of opportunities in this area.

John Tranquada asked if the specifications on the Multidimensional Atomic Resolution Electron Microscope could be achieved at the same time or if they would need to be done separately. **Zhu** shared that the goal is to achieve them simultaneously. The current instrument is not stable and he wants a stable stage for spectroscopy. This can all be done with one instrument. **Hall** added that the instrument idea that came out of the workshop shows that some capabilities are easier to achieve than others. He noted that there are tremendous implementation challenges and a five to 10-year timeframe for development. **Hall** noted that the goal with 3D and 4D tomography is to collect all of the scattering. How that would be done is unknown and that will take more development time.

Simon Bare noted that the atomic resolution microscope has enabled the understanding of materials. He asked if the workshop looked at the 'lab in gap' microscope as having other capabilities beyond just microscopy. **Zhu** shared that it is very hard to achieve a higher resolution. Electrons scatter strongly and the liquid cell is in a different state. If there is a high pressure in the gas chamber and you have extremely high resolution, then you can measure functionality. The workshop discussed chemical probes.

Zhu shared with **Chiang** that most of the natural microscopy in the 'lab in gap' tool is limited. People have used drops in gas chambers and graphene. You can use natural chemicals but there is an issue there. With the 'lab in gap,' electron induced radiolysis has to be dealt with. It is an evolving field but researchers are learning whenever they conduct this type of work.

PUBLIC COMMENT

None

BOARD BUSINESS

None

ADJOURNMENT

The BESAC meeting was adjourned by **Hemminger** at 10:15 p.m.