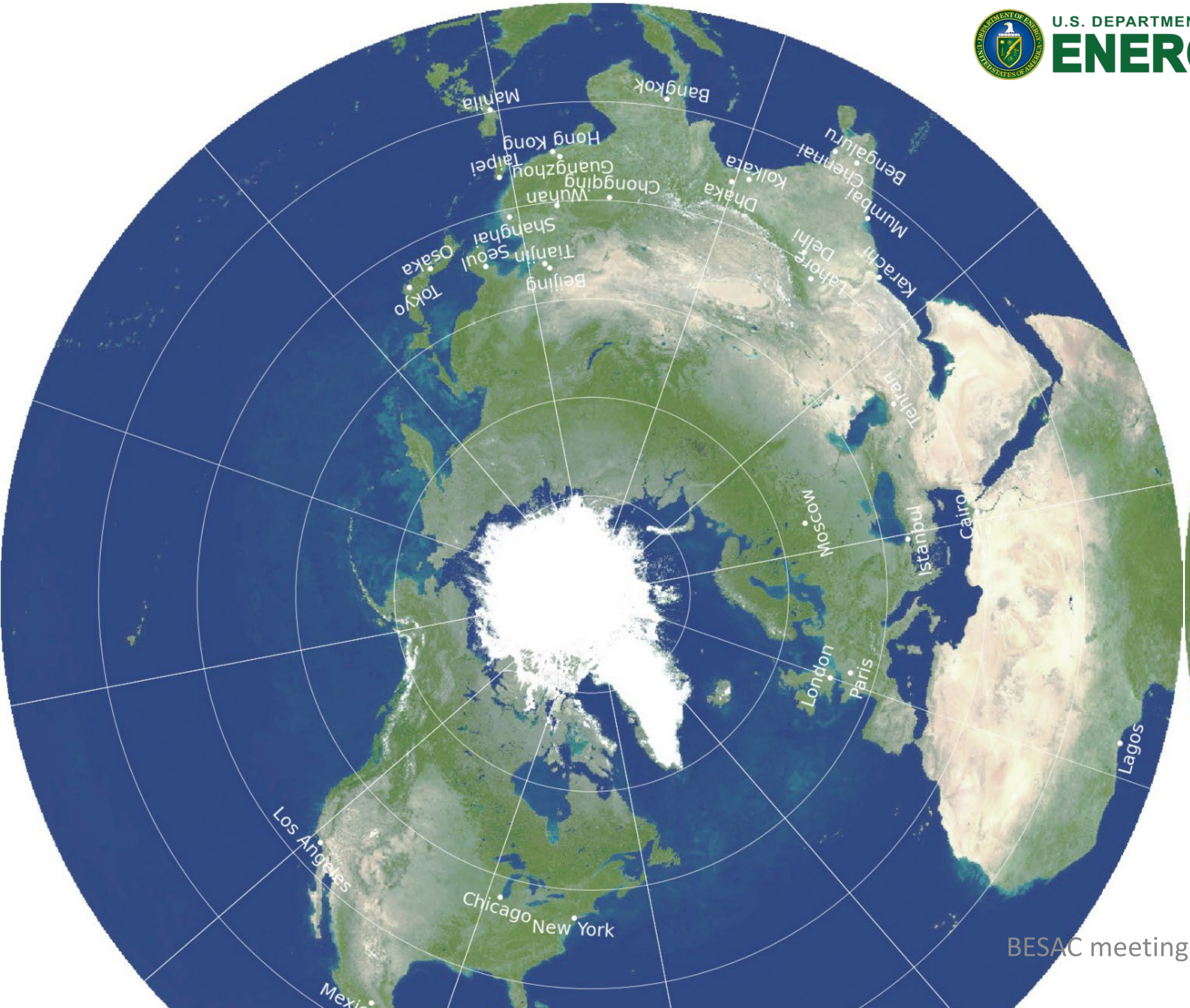
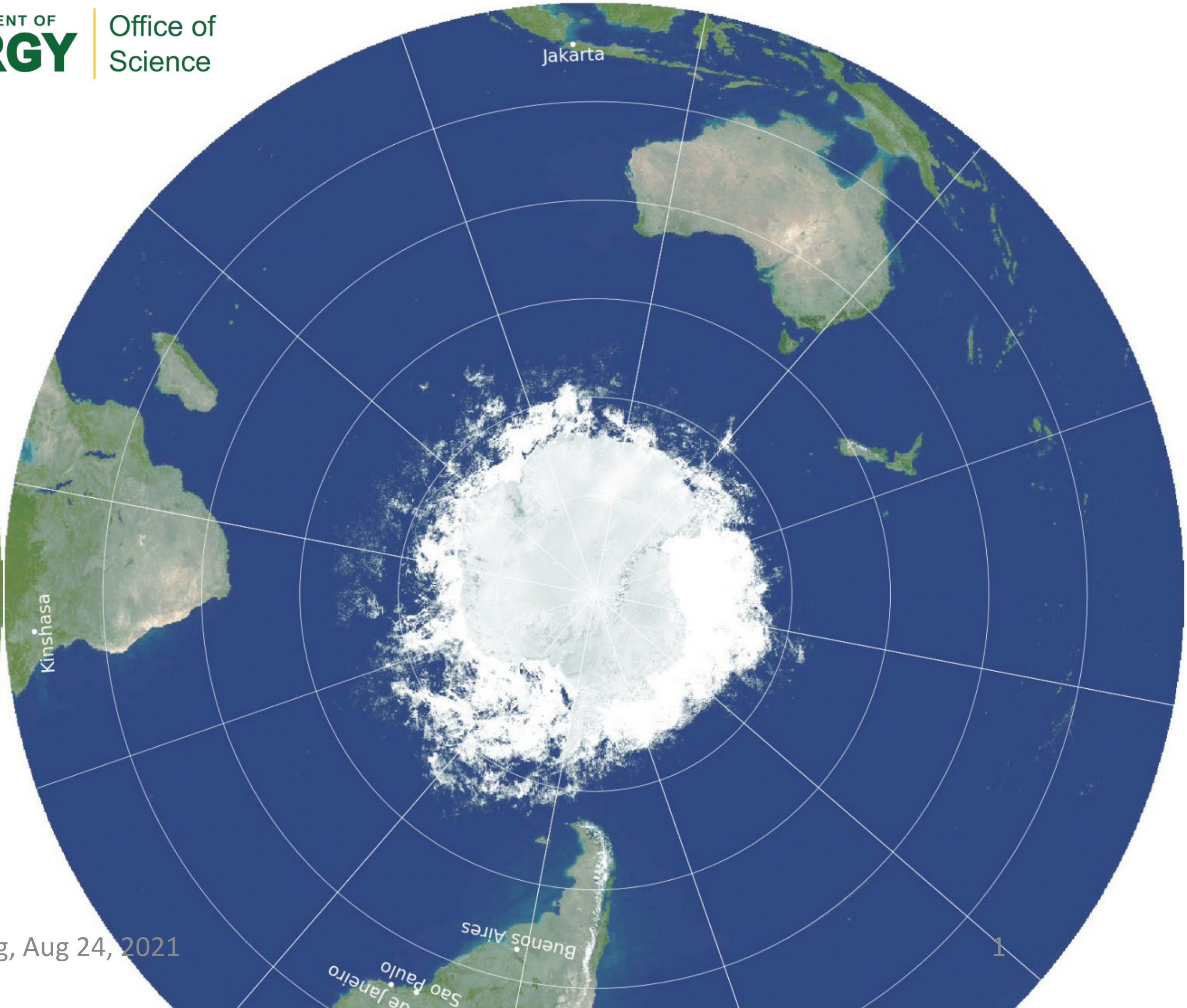
CAN THE U.S. COMPETE *in Basic Energy Science?*

Critical research frontiers and strategies

A report by the BESAC Subcommittee on International Benchmarking

U.S. DEPARTMENT OF ENERGY | Office of Science





Meeting Outline

- Charge
- Team
- Executive summary
- Key Findings and Recommendations
- Methodology
- The Stories
- Discussion

DOE Office of Science Charge to the Sub-committee
(summary)

1. to identify key areas of its mission-relevant research and facility capabilities in which U.S. leadership is most threatened,
2. to advise on modifications to existing trade-offs or new ways to leverage scarce resources,
3. to identify incentives that will retain and attract scientific talent.

International Benchmarking Subcommittee

Subcommittee Leads	
Chair **Cynthia Friend**	Harvard University
Vice Chair **Matt Tirrell**	University of Chicago
Team Lead **Eric Isaacs**	Carnegie Institution for Science
Team Lead **Zhi-Xun Shen**	Stanford University

BES Participants	
Linda Horton	Basic Energy Sciences
Thomas Russell	Basic Energy Sciences

Subcommittee members	
Frank Bates	University of Minnesota
Anthony Cheetham	UC Santa Barbara
Serena DeBeer	Max Planck Institute for Chemical Energy Conversion
Yan Gao	GE (Retired)
Brett Helms	LBNL
Marc Kastner	MIT (Retired)
Maki Kawai	Institute for Molecular Science
Y. Shirley Meng	University of California, San Diego
Pietro Musumeci	UCLA
Jüergen Mlynek	Humboldt University Berlin
Monica Olvera de la Cruz	Northwestern University
Abbas Ourmazd	University of Wisconsin – Milwaukee
Maria Santore	University of Massachusetts – Amherst
Eric Stach	University of Pennsylvania
Esther Takeuchi	Stony Brook
Birgitta Whaley	UC Berkeley

International Benchmarking Support

Logistics and Technical Support	
Katie Runkles	Basic Energy Sciences
Jeffrey Miller	Harvard University
Leah DeFrancesco	Harvard University
Tammy Click	ORISE
Al Hammond	Editor/writer
Maggie Powell	Publication design

Library Science Support
Tiffani R. Conner
Ann B. Gonzalez
Holly Holt
Jim Malone
Nathan Murray
Jennifer Tucker
Graphics support
Mike Dunner
David M. Goldberg
J. Richard Gott III
John Hill
Eric Johnson
Jeffrey Miller
Lisa Miller
Dennis Mills
Piero Panetta
Robert Schoelein
Robert J. Vanderbei

Executive Summary

Executive Summary

- Scientific discovery is a cornerstone of American prosperity
- The US has long been the leader in areas of research critical to BES
  - Especially in development of large-scale facilities
- Other nations are rapidly catching up and overtaking the US
  - Corresponds to rapid growth in research investment by China and EU, along with flattening US investment
- Without continued investment in basic science today, future discoveries and technological innovation will languish

Four Broad Strategies for Success

- Increase investment in basic energy sciences research
  - including the development of advanced research facilities and instrumentation.
- Boost support for early-career and mid-career scientists
  - so as to better attract and retain talent.
- Enhance opportunities for staff scientists at advanced research facilities
  - to provide for career development and talent retention
  - to unleash their creativity for instrumentation development and facility improvements.
- Better integrate energy sciences research across the full spectrum—from basic to applied to industrial research.

Critical Areas for Basic Energy Research

5 broad areas identified as critical fundamental scientific topics for leadership in BES

- These areas identified through analysis of BESAC reports and BRN reports
  - More methodology details later
- Only basic scientific research prioritized by Office of Basic Energy Research considered in report
  - Likely that trends apply to other fields of interest in energy science.

- All areas identified have potentially significant impacts on future US innovation and technology development

Critical Areas for Basic Energy Research

Area	Examples
Quantum Information Science	Quantum computation, quantum communication, quantum simulation, quantum sensing
Science for Energy Applications	Membranes, interfaces, energy storage, sustainable fuels
Matter for Energy and Information	Quantum materials, mesoscience, nanoscience, neuromorphic computing
Industrially-Relevant Science for Sustainability	Chemical upcycling of polymers, electrocatalysis, carbon capture, transformative manufacturing
Advanced Research Facilities	Neutron facilities, synchrotron and free electron X–ray sources, electron microscopy

Key Findings and Recommendations

Key Findings (1)

- Overall downward trend in all research areas from 2010 to present
  - Driven by increased investment in Europe and Asia, flat funding in US
- World-class research facilities, an important component of leadership
  - US facilities funded by BES are world leading
    - Long-range strategic planning
    - Ongoing stewardship and investment
  - US facilities no longer unique
- Mid- and small-scale instrumentation another cornerstone of science
  - New instruments built in individual labs historical led to breakthroughs (MRI)
  - Support increasingly difficult to obtain

Key Findings (2)

- Increasing importance of computation and data analysis
  - New hardware and software (codes, algorithms, AI, machine learning) critical to both science and technology
  - US is not leading overall in these areas
  - Concern for national security, science, engineering
- Competition for global talent
  - A historical US strength, now losing ground
- Need to facilitate overlap between basic, use-inspired, applied and industrial research
  - To shorten the time from discovery to application. (E.g., Coronavirus)

Recommendations

- Stronger investments in advanced research infrastructure
  - including laboratory-based and large-scale instrumentation
- Balancing the need to develop world-leading facilities and the need for access to and technical support of existing facilities
  - to increase research impact and help retain talented scientists.
- Mechanisms for significant financial support of scientific investigators at all career stages
  - to create a more sustainable career path that builds on current investments in the development of the scientific work force
  - to enhance U.S. competitiveness for talent.
- Additional investment in computational and data analysis methods, computer hardware and architecture
- Enhanced international cooperation in selected areas has the potential to enhance U.S. competitiveness.
- Facilitation of interaction across the continuum of basic research, use-inspired research, applied research and industrial research could accelerate translation of fundamental research to impactful technologies that benefit society.

Methodology

DOE BES Basic Research Needs Studies

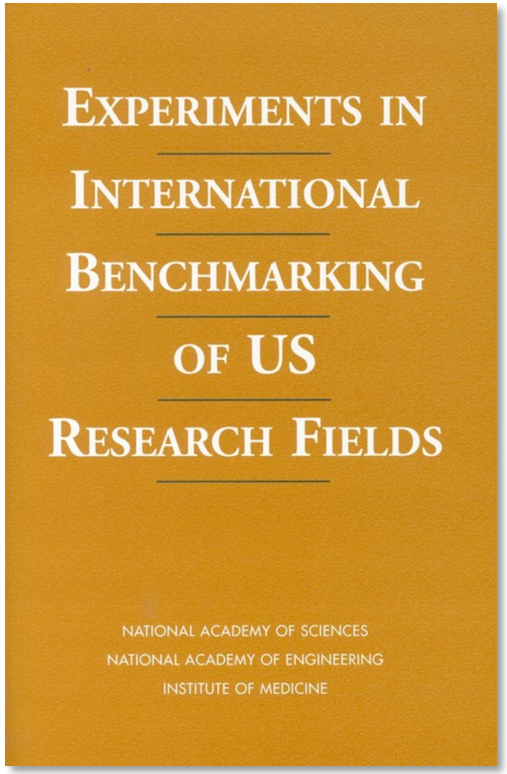
- Rationale for BRN use
  - Comprehensively describe BES priorities
- BRN reports back to 2010 considered
  - List of reports selected for further study →
- Areas selected based on strategic value to BES

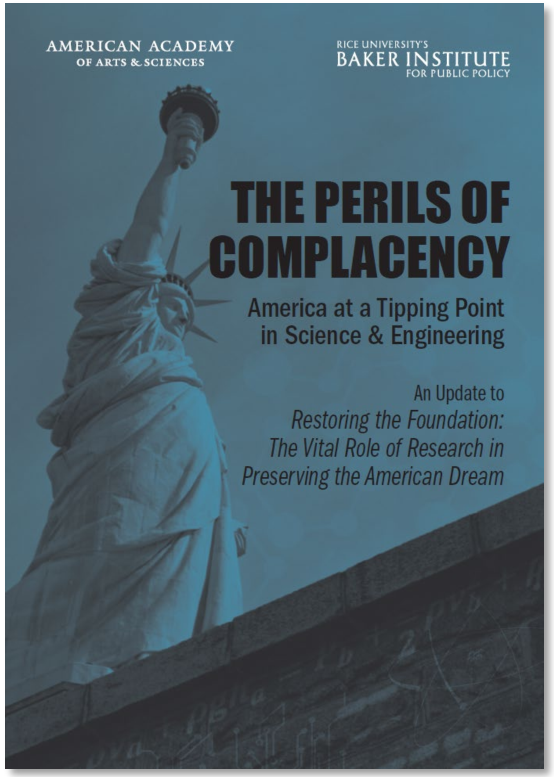
QIS	BES Roundtable on Opportunities for Quantum Computing in Chemical and Materials Sciences (2017)
	BES Roundtable on Opportunities for Basic Research for Next-Generation Quantum Systems –group with Quantum computing(2017)
Science for energy applications	BES Roundtable on Liquid Solar Fuels (2019)
	BRN for Next Generation Electrical Energy Storage (2017)
	BRN for Synthesis Science for Energy Technologies (2016)
	BESAC Report on Science for Energy Technology (2010)
	BRN for Energy and Water (2017)
	BES Roundtable on Sustainable Ammonia Synthesis – Exploring the scientific challenges (2016)
Matter for energy and information	BRN for Microelectronics (2018)
	BES Roundtable on Neuromorphic Computing – From Materials Research to Systems Architecture (2015)
	BESAC Report on From Quanta to the Continuum: Opportunities for Mesoscale Science (2012)
	BES report on Computational Materials Science and Chemistry (2010)
Industrially-relevant science for sustainability	BRN Workshop on Transformative Manufacturing (2020)
	BES Roundtable on Chemical Upcycling of Polymers (2019)
	BRN for Catalysis Science to Transform Energy Technologies (2017)
	BRN on Quantum Materials for Energy Relevant Technology (2016)
	BRN for Carbon Capture: Beyond 2020 (2010)
Advanced research facilities	BES Roundtable on Opportunities for Basic Research at the Frontiers of XFEL Ultrafast Science (2017)
	BRN for Innovation and Discovery of Transformative Experimental Tools (2016)
	The Scientific Justification for a U.S. Domestic High-Performance Reactor-Based Research Facility
	Future of Electron Scattering and Diffraction (2014)
	BES Workshop On Future Electron Sources (2016)

Areas, First Step: Review Previous Studies

Selected previous studies:

- NAS report on how to do benchmarking
  - Broad collection of expert opinion is a key to minimize bias
    - "Theoretical Congress" or conferences a way to obtain
- American Academy report





Based on these studies, the methodology was developed (next slide)

Methodology overview ("Team 1" : Areas)

1. Select Areas

Used BRNs and expertise of team to select strategic areas of importance to BES

Scientific Areas

Area 1
Area 2
Area 3
Area 4
Area 5

2. Rank the areas and select deep-dive areas

Discussions with experts and BRN leaders.

Expert ranking results

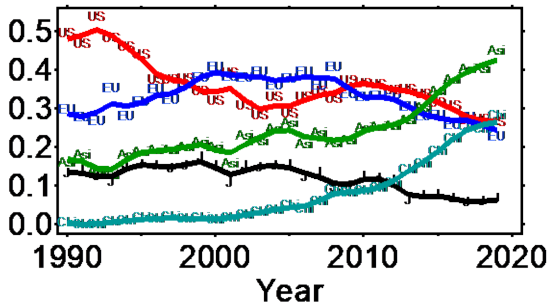
Expert ranking of areas	Current			Future		
	1	2	3	1	2	3
Example rank 1		●		●		
Example rank 2	●				●	
Example rank 3			●		●	

3. Analyze deep-dive Areas

Publication metrics (ORISE + committee)
Conference analysis (committee)

Scopus®

Quantitative ranking results



4. Previous reports and community input

Awards, other metrics and **community input**

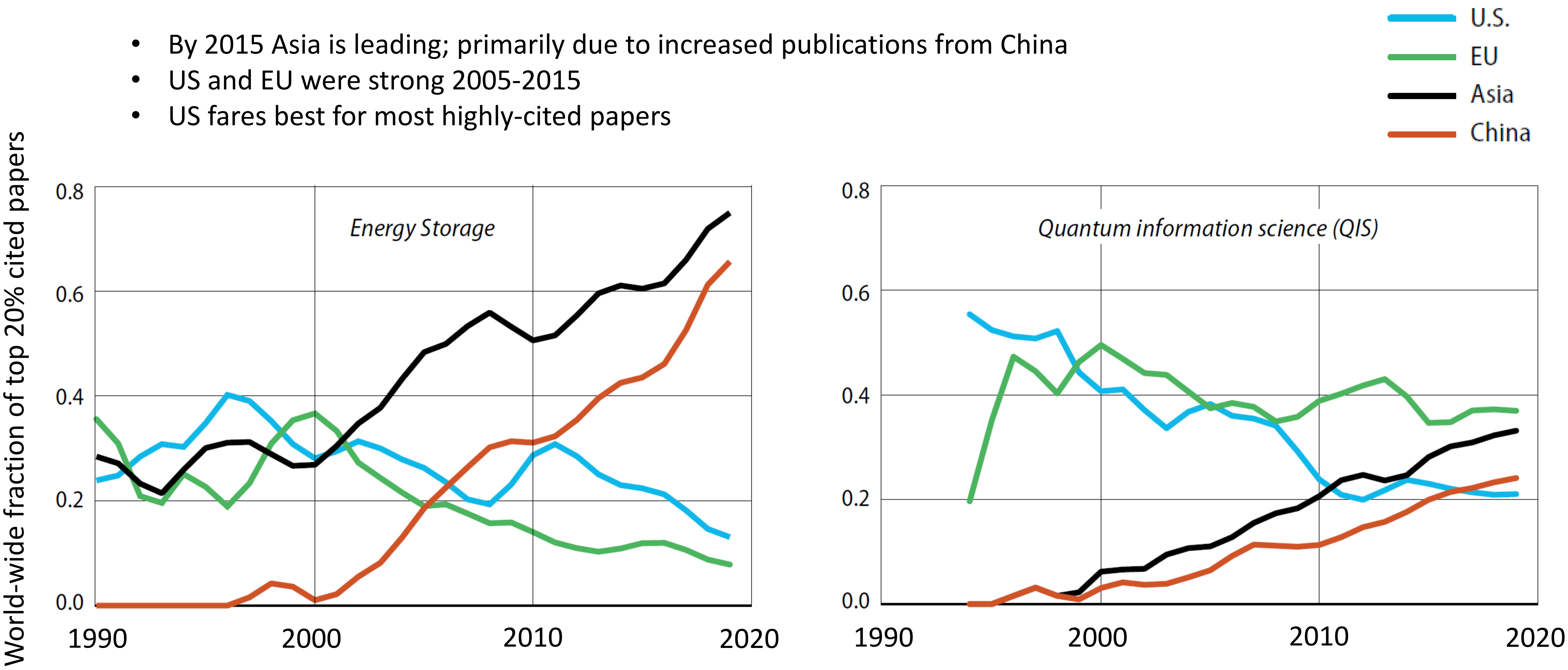
Webinars promoted by ACS, MRS, APS, ECS.

Consultation, conference & citation methodology

- Consulted with BRN chairs to understand perceived global status of the strategic areas
  - Selected sub-areas for deep-dive conference and citation study based on consultations
- Conference methodology
  - Generated lists of recent world-wide conferences in sub-areas
  - Enumerated invited speakers by nation/region
- Citation methodology
  - Generated keyword lists in sub-areas
  - Enumerated publications by nation/region, including effect of citation counts
  - Also studied international facilities use in top-cited papers

Selected Citation Results

- By 2015 Asia is leading; primarily due to increased publications from China
- US and EU were strong 2005-2015
- US fares best for most highly-cited papers



Increase in Chinese publications correlates with increased funding in China

Data for gross expenditures for *all* R&D

American Academy report “The Perils of Complacency,” Fig 1, p. 13

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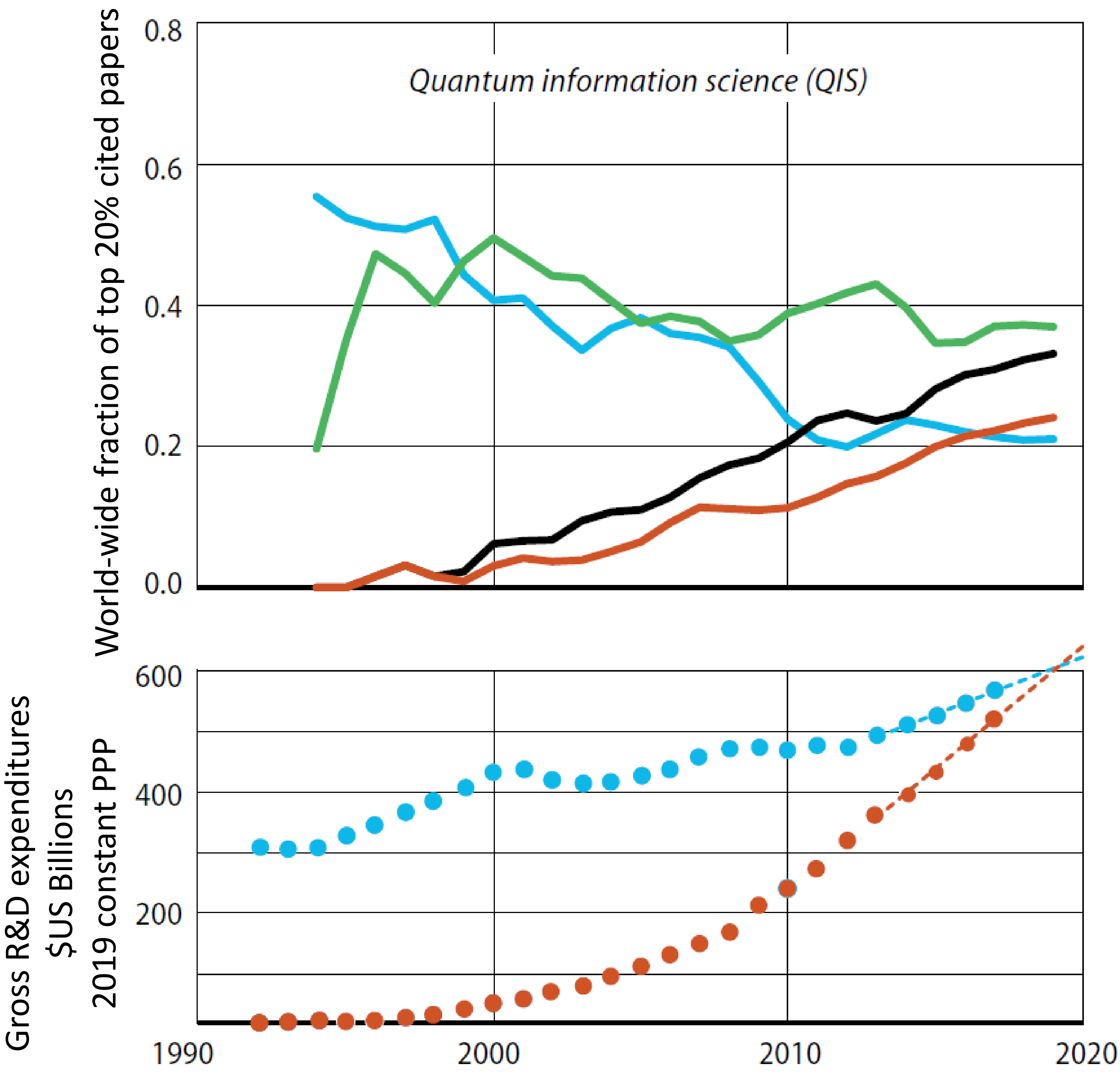


Methodology (“Team 2” : Strategies)

- Determined categories of consultants to contact
- Conducted over 50 consultations using a similar request-for-information tailored to categories
- Extracted hypotheses for key strategic themes
- Next Steps:
  - Seek input from science community at townhall meetings at APS (March), ACS (April 6), MRS (April 26), ECS (June 1)
  - Test hypothesis with additional consultations

Categories of consultations

- US Lab leadership
- NSF leadership
- Private foundation leadership
- University leadership
- International leadership in research, facilities and management
- Early career scientists (eg, DOE Early Career Awardees)
- US and international industry leadership

Hypotheses tested

- US is losing in global competition for talent.
- US facilities are excellent but European facilities provide better support for science programs and longer-term facility planning for future generations of scientists.
- Stronger investments in infrastructure are needed to bolster US competitiveness.
- Computation and data science capacity across fields seem to be lagging in the US.
- Larger financial support levels for early career investigators, and follow-on financial support for outstanding people to transition to mid-career, are needed.
- Enhanced international cooperation would in turn enhance US competitiveness.
- Facilitation of overlapping and mutual stimulation among basic research, use-inspired research, applied research and industrial research would invigorate the US system.

How to test hypotheses

- Thorough discussion among Team 2 as to the validity, comprehensiveness, and formulation of these hypotheses.
- Seek data supporting each of these hypotheses, if they exist.
- Develop anecdotes or compelling stories supporting each of these hypotheses, if possible.
- Pursue more pointed discussion with the sources of these hypotheses to explore them more thoroughly.
- Seek more sources to corroborate or refute specific hypotheses. Consider what other sources may be for this purpose.
- Assemble some real-time, on-line, panel discussions with source, including those previously consulted and some new ones.

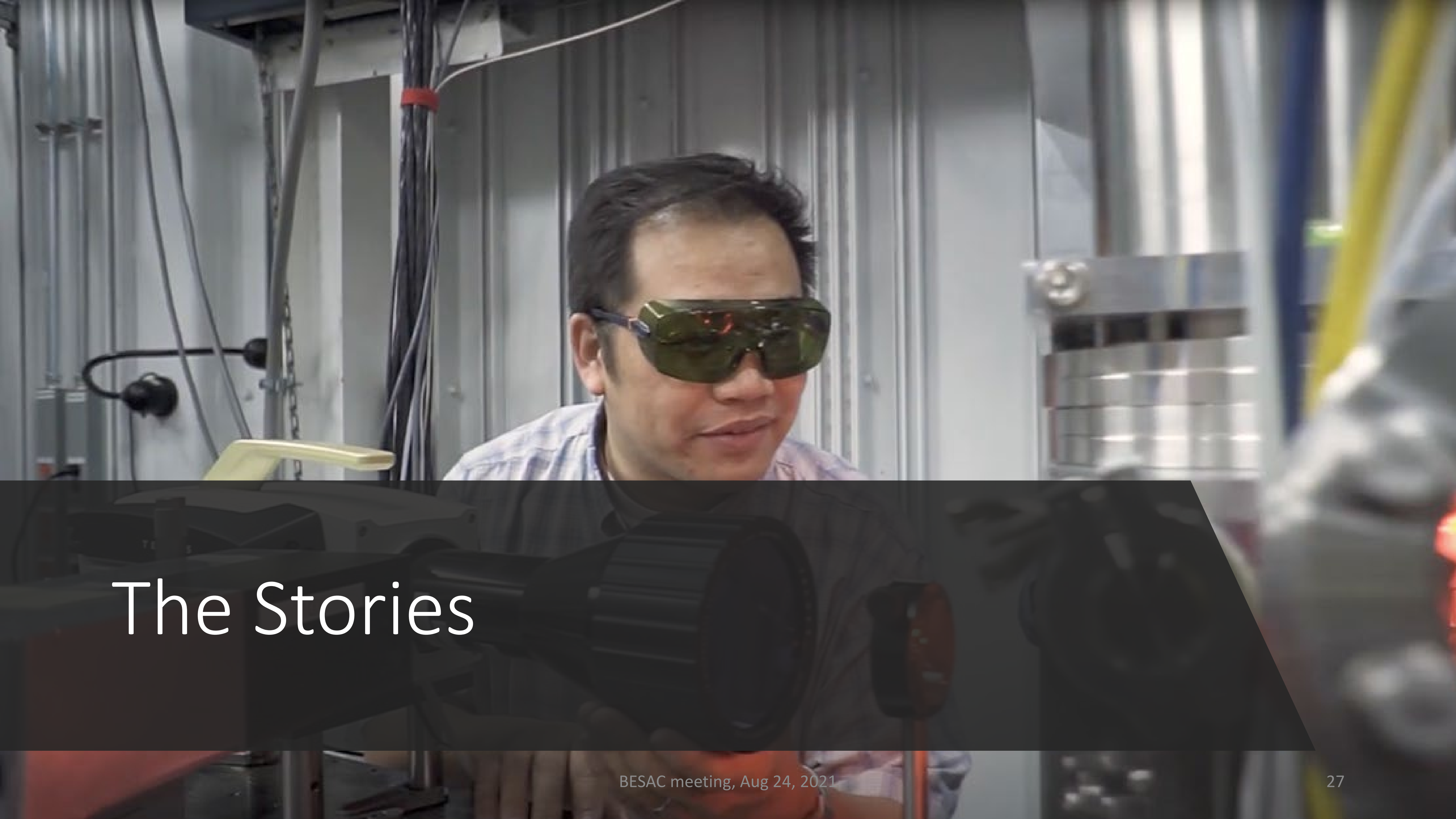
Additional facilities focused consultations with users, user organizations and user facility staff

1. What are some of the best management practices from the point of view of enhancing users' research at [facility name]?
2. Are there some management practices you would like to see improved from the point of view of enhancing users' research at [facility name]?
3. Does [facility name] continue to upgrade or develop state of the art instruments that enable world-leading research?
4. Does [facility name] enable/recruit top research talent as 'in-house' drivers of science and instrumentation?
5. Does [facility name] strike a good balance among the various goals of providing access to all qualified users, providing expert staff support to users, and pursuing strong science program collaboratively with users? Would you like to see the balance adjusted or improved in some ways?
6. Are you able to make any comparisons among different facilities, nationally and internationally, with respect to how each operates to enhance users' research?
7. What is the best facility world-wide for the kind of work that you do? (what is your field?) What makes it best?
8. How effectively do you think [facility name] plans for the future, in both the near-term and the long-term?

Additional facilities focused consultations
with users, user organizations and user facility staff

Some generalizations coming out of this round:

- Facilities with highest impact on science
  - Enable staff to think creatively and big, to develop new directions and tools
  - Provide intellectual engagement as well as expert help to users
  - Perform training and knowledge dissemination function
  - Develop a career environment for outstanding scientists
- There seems to be a general feeling that compared to international competition, US facilities are able to attract excellent people, but their time for research and the investment in the tools of the facilities are less.
- Interesting opportunities to enhance engagement between BES and accelerator science (HEP) in areas from electron microscopy to light sources.



The Stories

Story	Tools and facilities	Subject	Benchmarking message
A Testbed for Secure Quantum Communications	Argonne	Physics	The basic science of creating and controlling entanglement over long-distances, pertinent to quantum communications, with implications for how we think about both information and security; an instance where China and others are investing heavily.
Creating the chemistry for better, smarter materials	LBNL	Chemistry	Fundamental science to address looming environmental and supply challenges
Catalyzing a U.S. Manufacturing Revolution	Argonne	Materials	Fundamental research and technology transfer. Talent retention. Facilities availability.
Building a better battery for clean energy storage	LBL, ALS, novel tool	Chemistry	Coordination between national labs and the university-based innovation ecosystem yields both good basic science and economically promising ventures.
Transforming Structural Biological Science and Biomedicine	SLAC, XFEL, LBL, international	Chemistry	Strategic planning of basic science facilities by DOE and broad international collaboration are yielding fundamental new insights and, potentially, new sources of clean energy.
How Data-Driven Science Is Helping Combat the COVID Crisis	Cryo-EM, Machine learning	Chemistry	How DOE investment in basic tools and international collaboration can result in life-changing outcomes. And the emergence of data-driven science and AI/ML as an important basic research methodology.
Competitiveness in Quantum Materials		Materials	Demise of big industrial labs (Bell labs, etc) exposed US weakness in materials synthesis forcing reliance on foreign supplies, until a shift in the culture of physics departments resolved the problem.
Worldwide competition for talent	LBL, user support for soft neutron research	New tools	US can no longer take the international competition for talent for granted
Why Long-Range Planning is Critical to U.S. Competitiveness	SLAC, XFEL, LBL, international	Chemistry	Strategic planning of basic science facilities by DOE and broad international collaboration are yielding fundamental new insights and, potentially, new sources of clean energy.

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