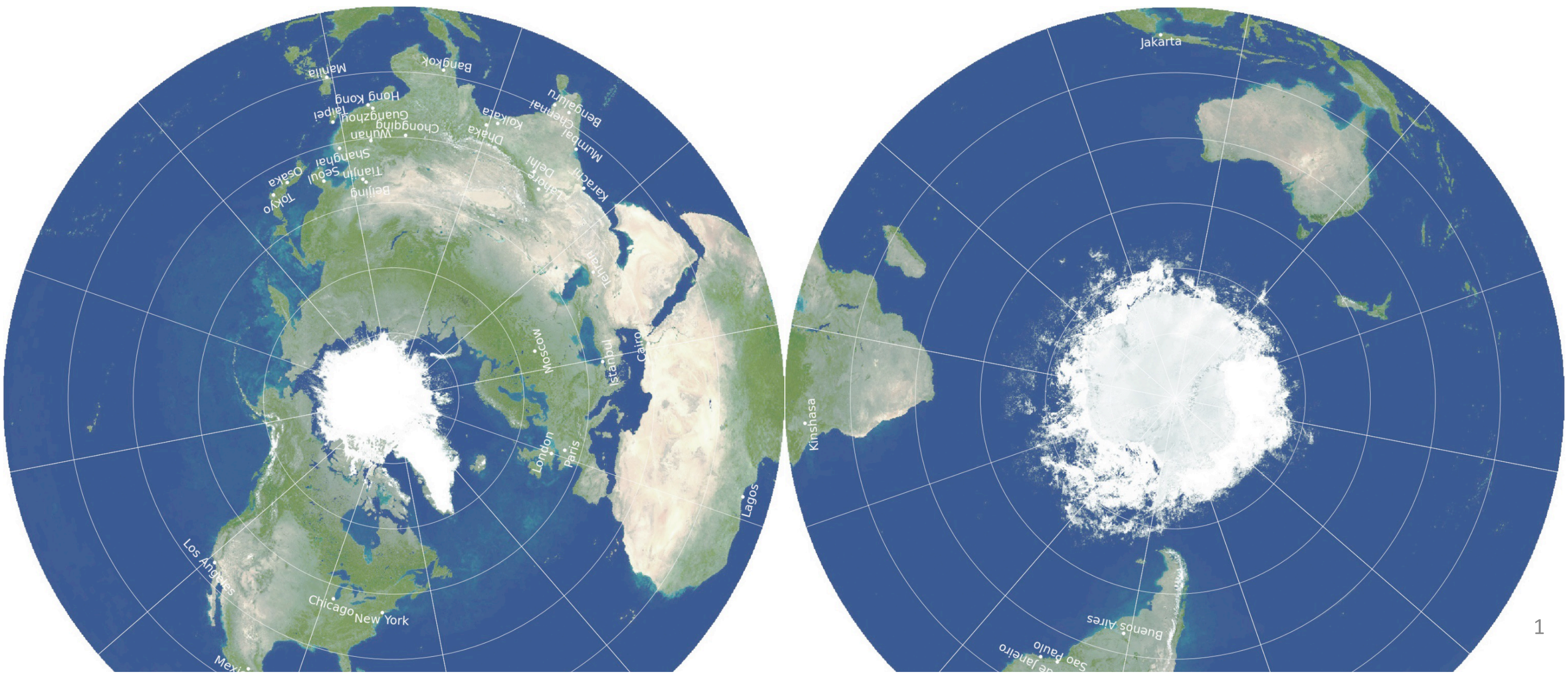
CAN THE U.S. COMPETE *in Basic Energy Science?*

Critical research frontiers and strategies

A report by the Basic Energy Sciences Advisory Committee (BESAC) Subcommittee

https://science.osti.gov/-/media/bes/besac/pdf/Reports/AH_DOE2021-International_Benchmarking.pdf



Report Summary

Findings

- An overall downward trend in competitiveness in all research areas
- U.S. advanced research facilities are no longer unique
- Support for mid- and small-scale instrumentation difficult to obtain.
- *The fierce global competition for scientific tal*ent

Possible Strategies for Success

- Increased investment in basic energy sciences research
- Additional investment in computation, data analysis methods, computer hardware and architecture
- Boost support for scientists, enhance U.S. competitiveness for talent
- Balance need for new facilities with support for existing facilities
- Better integrate research from basic to applied to industrial

Methodology

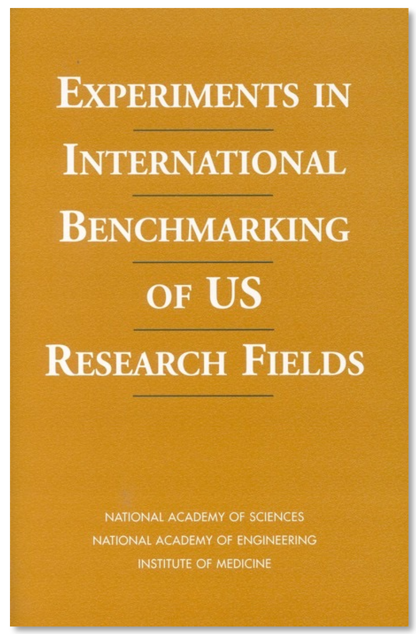
Researchers Emily Schroeder and Rosa Zelaya in the laboratory of Prof. Phil Christopher, UCSB and member of CCEI EFRC, use infrared spectroscopy to study function of innovative heterogeneous catalysts. (Credit: Lillian McKinney, UCSB)

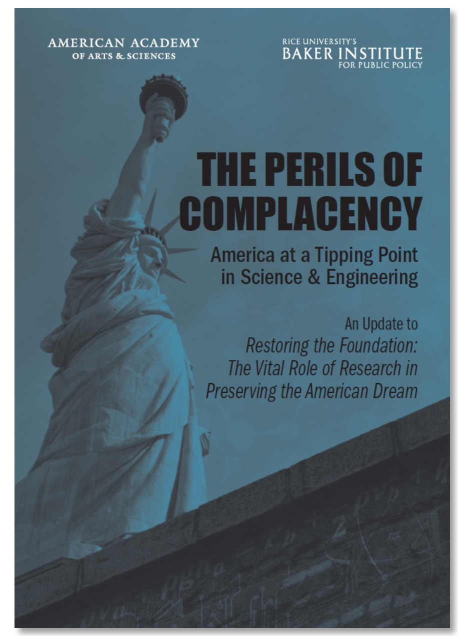
First step: review previous studies

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
    - National Academies Press, 2000, https://doi.org/10.17226/9784
- American Academy report
  - American Academy of Arts and Sciences, 2020, www.amacad.org/publication/perils-of-complacency.

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

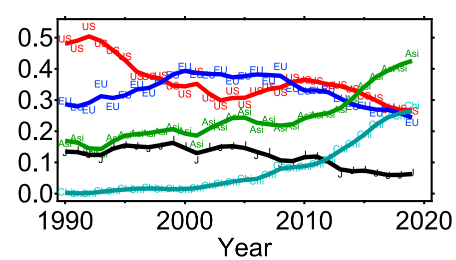
Expert ranking of areas	Current			Future		
	1	2	3	1	2	3
Example rank 1		●		●		
Example rank 2	●				●	
Example rank 3			●		●	

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.

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
  - Distilled to 5 areas, as also shown below.

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	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)
Materials 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)
Facilities/Cross-cutting	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)

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

Areas: Consultation, conference & citation methodology

- Consulted with BRN chairs to understand perceived global status of the strategic areas
  - Assessed and selected sub-areas for deep-dive conference and citation study based on consultations

Example: Ranking data from discussions with BRN leads

Area 5: Advanced Tools
Sub-Area: Neutrons, Reactor-based Research

	Current			Future			Researchers, emerging fields, other comments and insights
	1	2	3	1	2	3	
Neutron Scattering			●		●		Opinion 1. Behind Europe on sources and instrumentation but ahead of Asia. Potential to maintain position in the future provided DOE follows BESAC recommendations.
		●	●		●	●	Opinion 2. US significantly lags Europe and Asia-Oceania in neutron measurement capacity. The number of instruments available in US is much smaller than in other regions. In terms of capability the US is competitive in certain areas. However, in general the US lags Europe and J-PARC (Japan) in cold neutron and neutron diffraction capabilities Based on scientific output and impact the US community performs very well. Global leaders include: J-PARC, FRM-ll (Germany), ILL (France), ISIS (England) and ESS (under construction in Sweden).
Isotope Production	●			●			Opinion 3. There are only 2 reactors with flux greater than 1015 n/cm2s, required to produce critical isotopes, HFIR (ORNL) and SM-3 (Russia). The US will remain very competitive in this are provided HFIR is maintained.
Materials Irradiation	●				●		Opinion 4. Closure of 2 facilities, HALDEN (Norway) and OSIRIS (France) has left a shortage of neutron irradiation capability worldwide. Construction of the 100 MW JHR reactor in France, scheduled for completion by the end of this decade will help alleviate this problem and outcompete HFIR. However, if the US follows through on the Versatile Test Reactor, proposed by the DOE, this country will assume a highly competitive position in the study of materials under extreme conditions.

Current US position in this field
- 1-Forefront
- 2-Among world leaders
- 3-Behind world leaders

Likely future (5-10 years) US position
- 1-Gaining/extending
- 2-Maintaining
- 3-Losing Potential

The expert opinions are a critical component

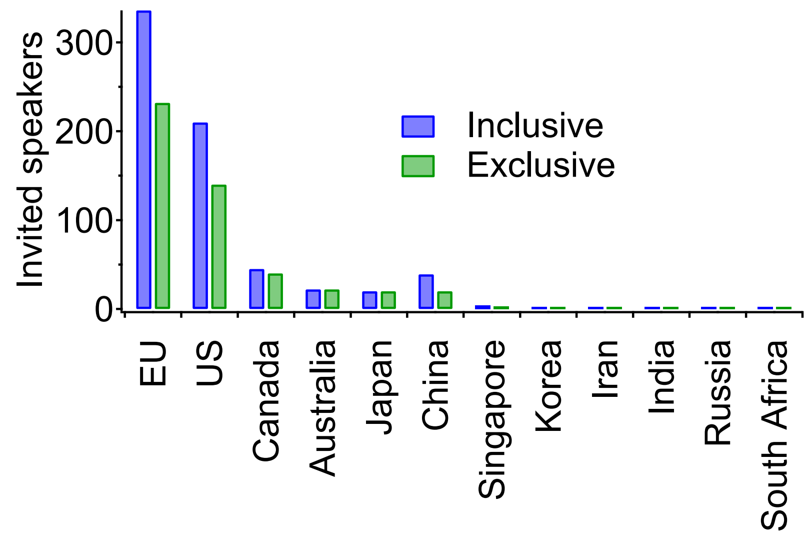
Conference methodology

- Conference methodology
  - Generated lists of recent world-wide conferences in sub-areas
  - Enumerated invited speakers by nation/region
- Consideration: Robustness of conference methodology
  - The method is semi-quantitative and interpretation requires judgement
    - No obvious way to include statistical uncertainty?
  - Is Asia appropriately captured?
    - Only English language conferences/journals considered?
    - Visa/Travel issues?
    - New/emerging experts not included in conference invitations?

Conference Methodology

- For all 5 areas, examined 78 conferences with ~2600 invited speakers
- Inclusive/Exclusive:
  - Effort to reduce “home field advantage,” doe we include speakers from home country or exclude?
- Representative result: Conferences on Quantum Information Science

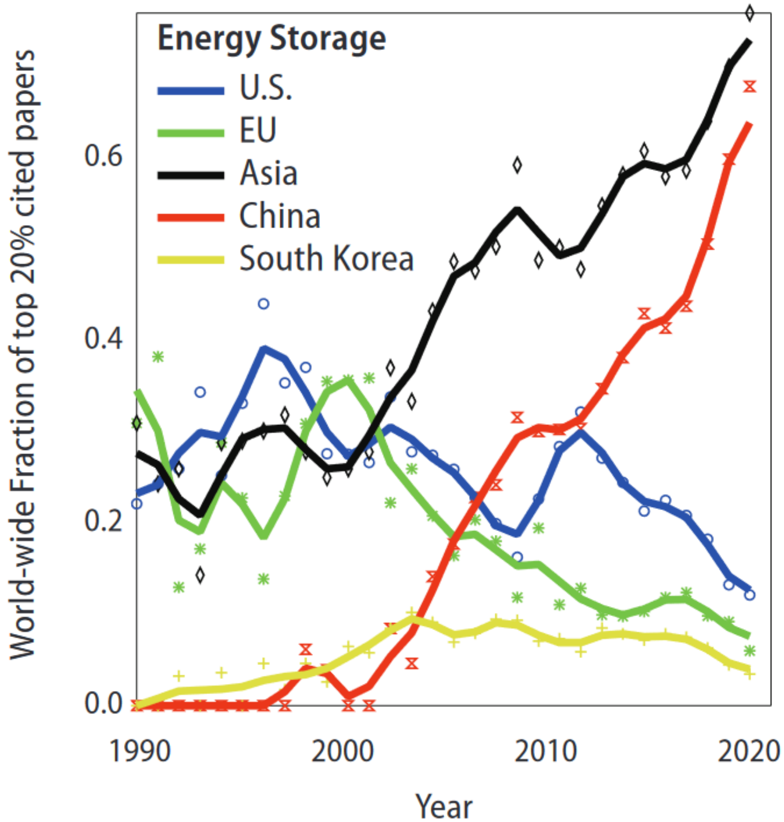
Country	Inclusive Count	Exclusive Count
EU	336	232
Asia	66	46
US	210	140
Canada	45	40
Australia	22	22
Iran	2	2
South Africa	1	1
Russia	1	1

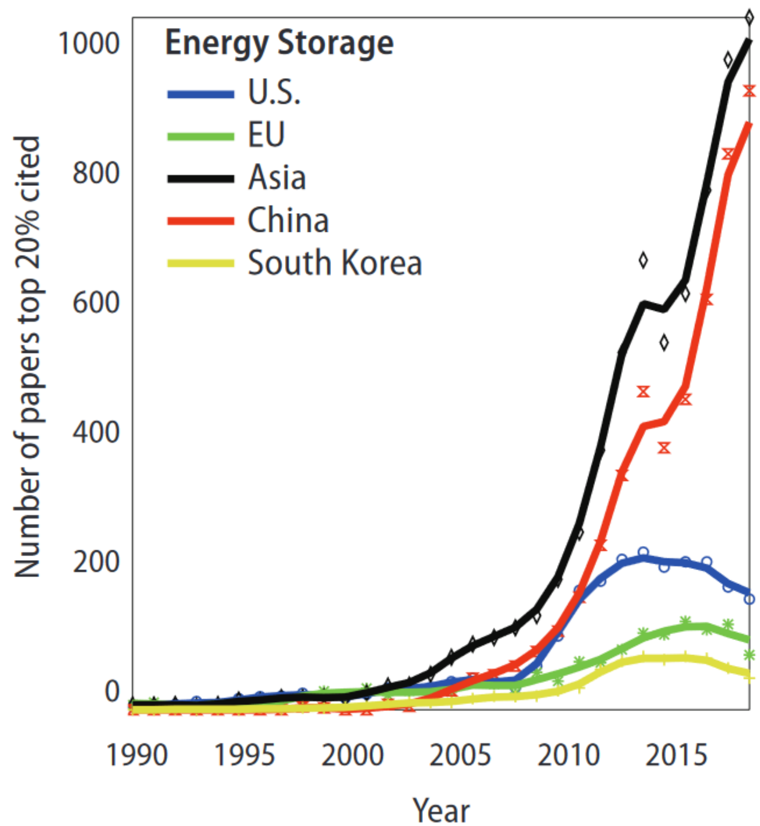


Citation methodology

- Generated keyword lists in sub-areas
  - Checked that "error rate" of "irrelevant" papers was <10%, or adjusted keywords accordingly.
    - Membranes: ({"reverse osmosis membrane"} OR {nanofiltration membrane} OR {ultrafiltration membrane}) AND ({polymer} OR {metal-organic framework} OR {covalent organic framework} OR {porous} OR {microporous}) AND ({water} OR {energy} OR {gas separations} OR {ion separations} OR {selective})
- Enumerated publications by nation/region and year (2010-2019), including effect of citation counts
- Also studied international facilities use in top-cited papers

Representative citation result



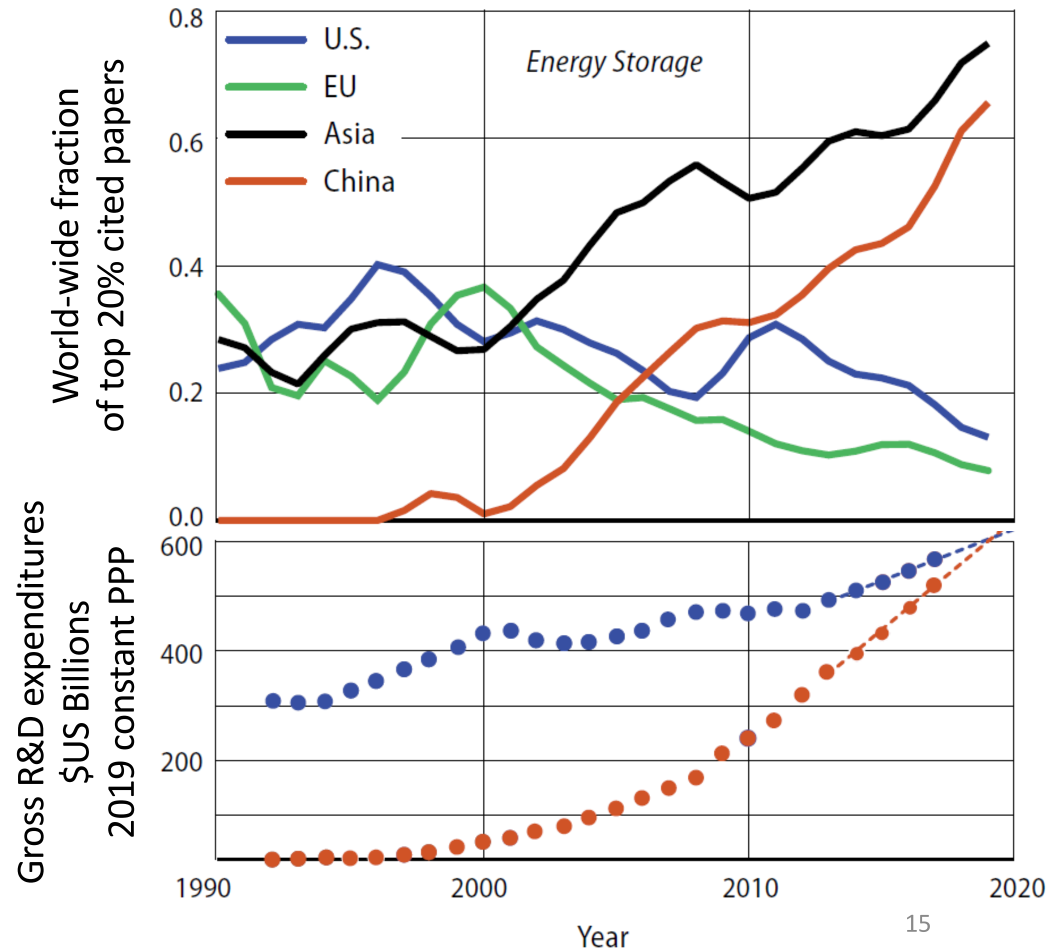


Markers are raw data, lines are a slightly smoothed guide to the eye

Other nations are catching up, overtaking the US

- Overall downward trend in competitiveness in all research areas, 2010-present
- Increased investment by E.U. and China; nearly flat U.S. funding.

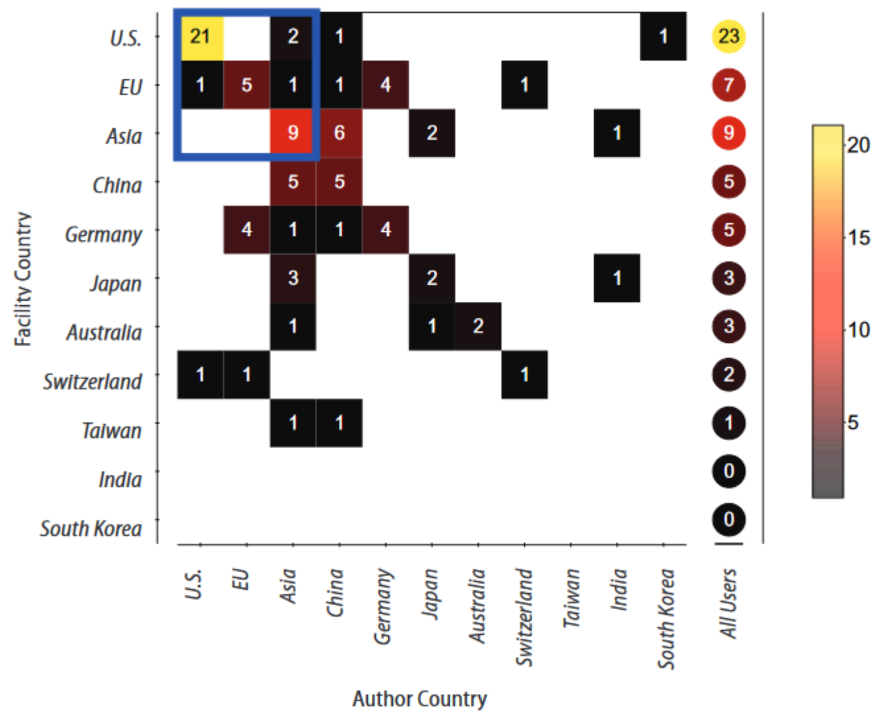
Similar trends found in other areas—see report



Expenditures data from *The Perils of Complacency, America at a Tipping Point in Science and Engineering* (American Academy of Arts and Sciences, 2020), www.amacad.org/publication/perils-of-complacency

Citations and cross-cutting facility locations

- Matrices were generated showing home country of authors vs. location of facilities.
  - Time-consuming method
  - Mainly showed that authors prefer nearby facilities.



Methodology for Strategies Team

What was done:

- Conducted over 50 consultations using a request-for-information
- Extracted hypotheses for key strategic themes
- Input from science community at townhall meetings at APS, ACS, MRS, ECS
- Follow up with additional consultations

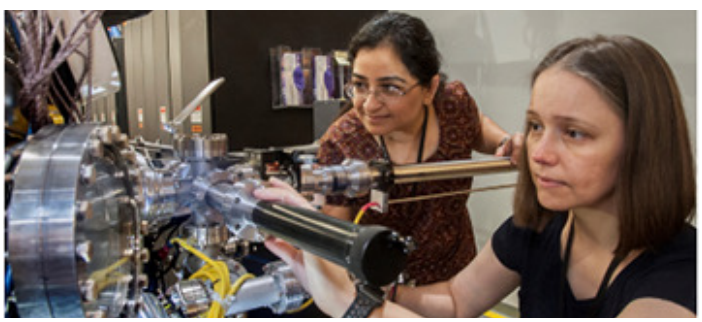


Photo credit: Brookhaven National Laboratory

Who was consulted:

- 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.
- Consider assembling 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?

The Stories

- The committee selected 9 side-bar stories
  - Selected to emphasize important findings or points from the report
  - Add more “human interest” or “real world” value to the report
    - Target audience is not necessarily highly technical

- A representative collection of photos also selected
  - Adds color and interest to the report
  - Highlight important concepts
  - Selected to be inclusive across facilities and researchers

“Town Hall” Meetings

- Venues
  - ACS, APS, MRS, ECS
- Process
  - Present slides deck containing following:
    - The overview material, including charge, approach, subcommittee members,
    - A short description of methodology
    - Some preliminary results
    - A list of stories
    - Time line for report
  - Solicit feedback

International Benchmarking BESAC Subcommittee

Team of subject-area experts and experienced administrators with international experience.

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Vice Chair **Matt Tirrell**	University of Chicago
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