Updates on International Benchmarking Study

- Charge
- Timeline
- Team/Report organization
- Progress update
  - Scientific Areas (Team 1)
    - Leads: Cynthia Friend, ZX Shen
  - Strategies for leadership (Team 2)
    - Leads: Matt Tirrell, Eric Isaacs
- Input/Questions/Discussion

International Benchmarking Subcommittee

Subcommittee	
Frank Bates	University of Minnesota
Anthony Cheetham	UC Santa Barbara
Serana DeBeer	Max Planck Institute for Chemical Energy Conversion
Cynthia Friend	Harvard University
Yan Gao	GE (Retired as of 10/30)
Brett Helms	LBNL
Eric Isaacs	Carnegie Institute
Marc Kastner	Retired MIT
Maki Kawai	Institute for Molecular Science
Y. Shirley Meng	University of California, San Diego
Pietro Musumeci	UCLA
Juergen Mlynek	Humboldt University Berlin
Monical Olvera de la Cruz	Northwestern University
Abbas Ourmazd	University of Wisconsin - Milwaukee
Maria Santore	University of Massachusetts - Amherst
ZX Shen	Stanford University
Eric Stach	University of Pennsylvania
Esther Takeuchi	Stony Brook
Matt Tirrell	University of Chicago
Birgitta Whaley	UC, Berkeley

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

Logistics and Technical Support	
Al Hammond	
Jeff Miller	Harvard University
Tammy Click	ORISE
Leah DeFrancesco	Harvard University
Katie Runkles	Basic Energy Sciences

Brief summary of Charge to the committee

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.

Timeline

By the end of the meeting in this month	Complete these tasks
August 2020	Identify key topics for study; begin data collection
November 2020	Gathering, analyzing, synthesizing data, redirecting inquiries as appropriate; Report out at BESAC meeting
December 2020	Agree on report outline
January 2021	Integrate data, ideas, recommendations. Write section outlines
Feb. 2021	Preliminary drafts of sections; preparation of interim report to BESAC
March 2021	Report to BESAC; modify report based on BESAC input
April 2021	Draft sections complete
May 2021	Draft report complete; handoff to Al Hammond
June 2021	Review Al Hammond's edits, provide feedback
July 2021	Report to BESAC for consideration of final report approval; submit report

Working Outline of Report

1. Front matter, including charge, subcommittee membership
2. Table of Contents
3. Executive summary
4. Introduction with global summary of context; *brief* summary of methodology
5. Stories to create interest and context—up to 10 interspersed in report
6. Critical areas for leadership
7. Strategies for Success
8. Facilities
9. Conclusions
10. Appendices
    a. Methodology
    b. List of sources
    c. References

Team leads to take primary responsibility for writing. Input from subcommittee members will be sought.

Team 1 (Scientific Areas) Progress Report

Friend, Shen

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

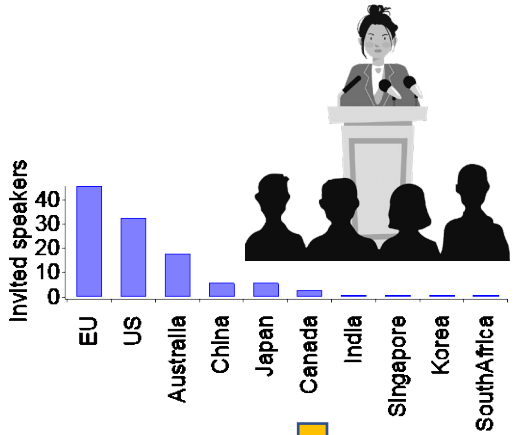
Discussions with experts and BRN leaders.

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

Conference analysis



Conference ranking results

Conference rankings of sub-areas			
	1	2	3
Example rank 1	●		
Example rank 2			●
Example rank 3		●	

4. Awards, other metrics, and community input

Awards, other metrics and community input

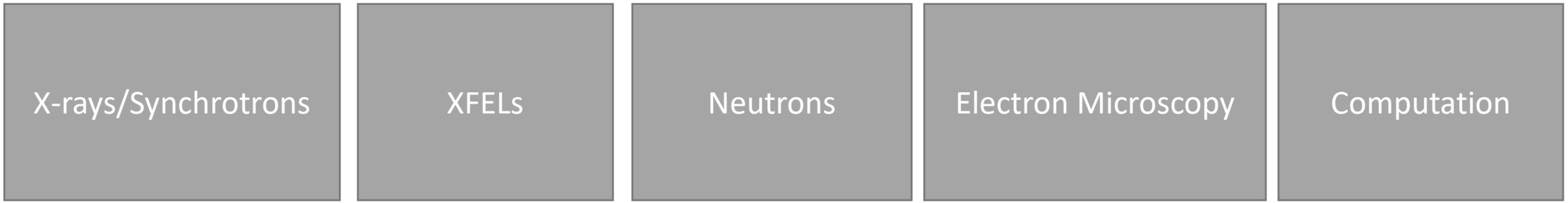
(In development)

The Scientific Areas

Area	Leads	Examples
1. Quantum Information Science	Shen and Whaley	Quantum algorithms, quantum computation
2. Science for Energy Applications	DeBeer and Santore	Membranes, interfaces, sustainable fuels
3. Innovative use of Matter for Energy and Information	Kastner and Meng	Quantum materials, mesoscience, nanoscience, neuromorphic computing
4. Industrially-relevant science for sustainability	Friend and Olvera de la Cruz	Chemical upcycling of polymers, electrocatalysis, carbon capture, transformative manufacturing
5. Advanced Tools (Cross-cutting)	Bates and Stach	Neutron facilities, XFEL, electron microscopy, light sources

Advanced tools: three critical components to evaluate

- Technical specifications of facilities
- Technical support/Access to facilities
  - (Addressed by Team 2)
- Scientific impact of facilities
  - (Developing approach to capture correctly)



Example: Ranking data from discussions with BRN leads

4. Industrially-Relevant Science for sustainability

	Current			Future			Summary of Expert Opinions *The expert opinions are a critical component*
	1	2	3	1	2	3	
BRN Workshop on Transformative Manufacturing (2020)							Not yet evaluated—preliminary report
BES Roundtable on Chemical Upcycling of Polymers (2019)		●			●		EU and US are both in leading position.
BRN for Catalysis Science to Transform Energy Technologies (2017)		●			●		US and EU in leading positions. US probably leading in electrocatalysis. China is rising in all areas of catalysis. New materials and focus on interfaces is important.
BRN for Carbon Capture: Beyond 2020 (2010)			●			●	US not leading. Comprehensive approach including separations and catalytic conversion needed. 2017 Mission Innovation report updates status from 2010 BRN.

Current US position in this field internationally
- 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

Conference Methodology (so far)

Methodology is evolving to minimized bias and ensure an objective data-based outcome

"Inclusive Count" (clear bias identified in this method)

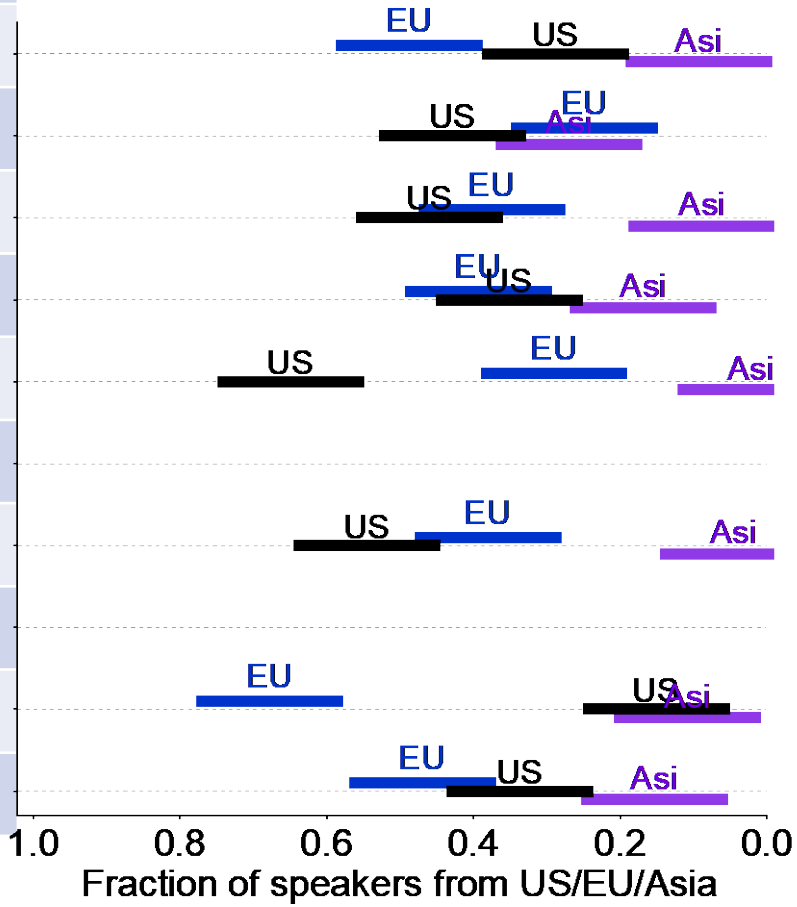
- Count all invited speakers from all conferences
- If speaker appears at more than one conference, count more than once.

"Exclusive Count" (less-biased method)

- Exclude speakers if they are speaking in their home country, unless we know the organizing committee has at least ½ of the members from non-home countries.
  - Certain conferences (Gordon, QIP, IMC) are organized by an international committee and so we do not exclude home-country.
- Speakers from *any* EU country are excluded from EU conferences
  - EU includes UK, Israel. Not Russia.

Conference Analysis Summary (Provisional)

Deep-dive sub-area	Impression from conference analysis		
	1	2	3
1. Quantum Information Science		●	
2. Membranes and Interfaces : synthesis and characterization		●	
2. Sustainable fuels including solar/electrochemical		●	
3. Quantum Materials		●	
3. Mesoscopics/Nanoscience	●		
3. Neuromorphic Computing			
4. Science for value-added reuse (chemical upcycling)		●	
4. Transformative Manufacturing			
5. Neutron Scattering (does not include all scientific impact)			●
5. Electron Microscopy		●	



(Exclusive counts)

●1-Forefront ●2-Among world leaders ●3-Behind world leaders

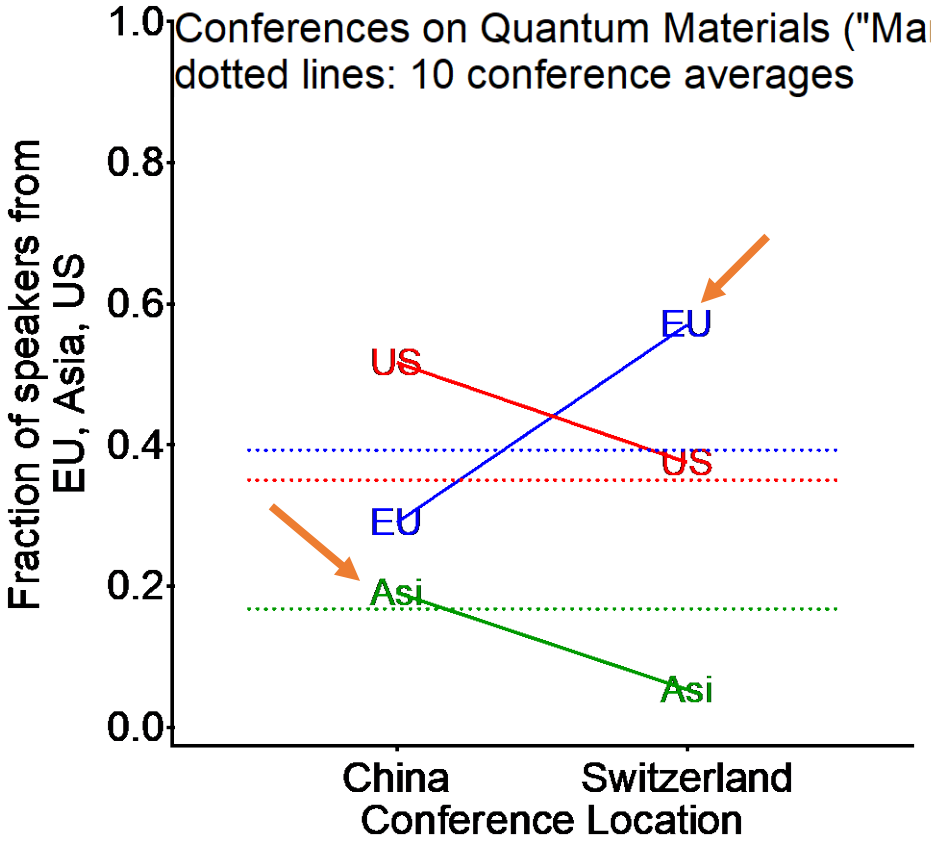
Is the conference methodology robust?

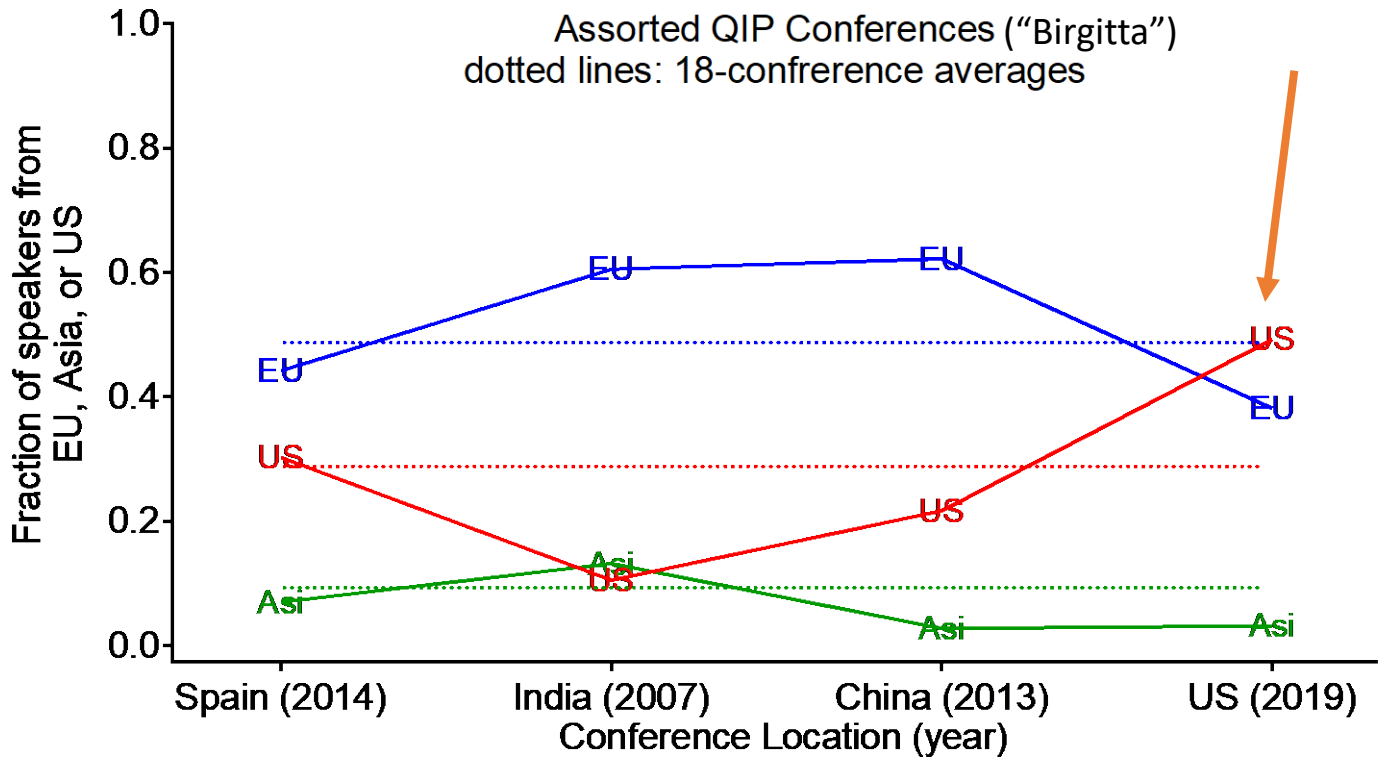
- The method is semi-quantitative and interpretation requires judgement—not subject to statistical analysis
- Is Asia appropriately captured?
  - Only English language conferences/journals considered?
  - Visa/Travel issues?
  - New/emerging experts not included in conference invitations?

Results from some initial “spot checks” performed—next slide

Effect of conference location “spot checks”

- *Qualitative* outcome is the same
- Some possible evidence of “home field advantage” but this should be largely corrected by “exclusive count”.





Citation “spot check”: Speakers selected from conferences—publication citations were analyzed by country of citation (per Web of Science)?

“Home field advantage” evident in citations. This is corrected in conference data

Author	Home Country	Conference Country	(Data set)	Citations		
				EU (%)	Asia (%)	US (%)
Thomas Jennewein	Canada	China	Whaley	39	13	4
Chao-Yan Lu	China	Italy	Whaley	39	49	7
Bernhard Keimer	Germany	Japan	Kastner	63	13	12
Zhi-Xun Shen	US	Japan	Kastner	23	29	46
Ady Stern	Israel	China	Kastner	71	4	23
Hai-Hu Wen	China	Switzerland	Kastner	6	76	16

Conference data		
EU (%)	Asia (%)	US (%)
48	9	30
39	17	35

Another citation spot-check

Clareivate Web of Science “Highly Cited Researchers 2020” report is qualitatively consistent with findings.

Country/Region	Percent of highly-cited researchers*
US	41%
EU	>23%
China	12%

*for all science fields, top 10 countries only, comprising 84% of highly-cited researchers

https://clarivate.com/webofsciencegroup/highly-cited-researchers-2020-executive-summary/

Interim summary of Team 1 results

- Data and analysis generated from consultations and from conference analysis
- Additional data analysis underway that also includes prizes
- Data sometimes does not agree with expectations of the team members based on their knowledge of fields
- Clear “homefield advantage” for conferences and citations
- Other evaluation methods need to be considered
- ***Broad community input is still needed***

Team 2 (Strategies) Progress Report

Tirrell and Isaacs

Team 2 Roadmap

1. Decide on categories of consultants to contact (done)
- Determine who would address each category (done)
- Discuss and refine questions to ask each category of consultant

2. Begin to contact consultants (done)
- Use a similar "request for information" tailored to category
- Report results (ten or more contacts made so far)

- Different questions asked of e.g., NL directors vs Early Career awardees
- Questions deal with strategies, mechanisms of advancing fields chosen by Team 1

Categories of consultants: a. leaders of national and. international research organizations, b. people with international and US experience, c. research center leaders, d. foundation heads, e. NL leadership, f. selected university leaders, f. Early Career awardees.

3. Extract key strategic themes (done)
- Compare responses seeking generalizations about successful strategies
- Distill into actionable recommendations

Articulate reasons
- What are the data, supporting arguments, experiences, …, that underpin these generalizations?

4. Present results at Nov 17 team 2 meeting (done)
- Before next meeting, exchange notes of consultation calls
- Discuss preliminary hypotheses and how to test those hypotheses

5. Next steps (after Nov 17 meeting)
- Additional consultations and data as needed
- Preparation of materials for Dec 10 BESAC meeting

Over forty telephone consultations

- **National Lab leadership**
- **NSF and private foundation leadership**
- **University leadership**
- **International leadership in research, facilities, and mgmt**
- **Early career scientists**
- **Domestic and international industry leadership**

Hypotheses to be tested

- US is losing in global competition for talent. See Tony Cheetham paper.
- US facilities are excellent but European facilities provide better support for science programs and long-term facility planning for future generations of scientists. See numerous call notes.
- Stronger investments in infrastructure are needed to bolster US competitiveness. See numerous call notes.
- Larger financial support levels for early career investigators, and follow-on financial support for outstanding people to transition to mid-career, are needed. See Brett Helms/Pietro Musumeci notes and Tony Cheetham paper.
- Enhanced international cooperation would in turn enhance US competitiveness. Several call notes.
- Facilitation of overlapping and mutual stimulation among basic research, use-inspired research, applied research and industrial research would invigorate the US system. Numerous call notes.

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.

Interim summary of Team 2 results

- Several important areas of concern have been identified (our hypotheses).
- Thus far, these are more in the realm of “diagnoses” rather than recommended “therapies”
- Further analysis and consultation will be done to lead toward recommendations.
- Some effort will be directed toward startegies for success in fields studied by Team 1.

Ways to get community feedback

- Reviewers of draft report
- Arranging meetings through scholarly societies (online)
- Web page with results and opportunity for input

Discussion

- Means of obtaining broad community input
- Possible changes in process or methodology
- Tentative plan for future meetings

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Thank You!