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Executive Summary

Responding to the request for strategies to guide the DOE Office of Science and, within that office, Basic Energy Sciences (BES), in making future investments in basic research, this report takes note of significant changes affecting the research environment. These include major advances in instrumentation that offer new research opportunities, such as X-ray and neutron sources; also the increasing cost of research as well as enhanced international competition, among other constraints. This report also recognizes the rapid evolution of machine learning and artificial intelligence tools that can potentially assist in research portfolio evaluation.

We believe that the Basic Energy Sciences program has an excellent track record in managing its research investments. Nonetheless, in the current context, we also believe that it is increasingly important for DOE, and Basic Energy Sciences (BES) in particular, to optimize its strategic research portfolios; to increase coordination within BES and with other programs; to expand resources to fund new opportunities; and to provide program managers with more flexibility. This report notes the success of periodic DOE reports on Basic Research Needs and encourages this and other efforts to communicate research priorities.

Based on numerous discussions with BES leadership, with National Laboratory directors, and with BES-funded researchers, this report finds that engagement with the research community is a cornerstone of BES success. We note with approval continuing efforts to create "low barrier" outreach efforts. At the same time, we believe there are significant opportunities for broader community engagement, and that the use of big data analysis and machine learning/artificial intelligence (AI/ML) tools should be cautiously considered, perhaps in partnership with other agencies.

We considered the important role U.S. industry can play in both the identification of new research areas and in translating the relevance of basic science insights to existing or new technologies. Thus, efforts to convene the community should continue to be inclusive of industrial researchers to align U.S. competitive needs. Dialog between industrial R&D efforts and the basic science community is also integral to the identification of pathways to enable translational research efforts. As an example, the scientific foundation of advanced manufacturing is important for U.S. competitiveness. This requires understanding of existing industry practices, as well as understanding how and why different basic R&D activities have impacted U.S. industry—and is critical to ensuring that the DOE's U.S. competitiveness mission can succeed.

Another important opportunity is the potential for partnerships with publishers, since dissemination of basic R&D discoveries is a critical activity. To date, the primary mode of dissemination has been peer-reviewed publications. Understanding the broader impact of research publications potentially aligns with publishers' efforts to understand their audiences. Thus, a partnership to track and share citations of publications and their impact might be feasible, and could enable advanced analytics to assess the impact of R&D investments, the balance of a portfolio across topics, and modalities such as single investigator or large team projects.

Analysis of research impacts and utility of the data generated by basic R&D remain a critical objective. The extent to which advanced data analytics, such as machine learning and artificial intelligence, can be used to make these assessments is a new and rapidly evolving area—which creates a potential

opportunity for DOE/BES to examine how data should be structured to enable such tools. This will enable DOE/ BES to consider AI/ML analysis tools including possible partnerships across agencies to facilitate adoption.

We analyzed the substantial existing literature on research assessment—in particular, research portfolio analysis (not single principal investigator assessment)—as a source of insights applicable to broader portfolio evaluations within DOE/BES. We find that publication metrics, especially when used in a nuanced and balanced approach, provide quantitative data that can gauge the influence and reach of research outputs. Such objective metrics allow responsible research evaluation and mitigate biases possible within peer review processes. However, the literature is clear that such metrics should be coupled with the informed judgement of domain experts and need to be normalized across different disciplines.

We recommend that the goals of a portfolio be clear, well-defined and assessable, and widely communicated. They should also be assessed for investment balance (such as between national laboratories and academia) and should be evaluated with both quantitative and qualitative metrics. Key data can also be gathered from sources such as funding acknowledgements, patent applications, and workforce development. Training tools are important to ensure accurate implementation of any research portfolio assessment system.

As portfolios within BES sub-disciplines mature, it is useful to verify that scientific foundations have been laid that sustain growth of new science fields, and to assess whether existing research programs continue to advance scientific knowledge and leadership with demonstrable impact. Thus, we find that portfolio analysis emerges as an important tool for the Office of Science, helping to ensure that resources are being allocated efficiently and effectively. Portfolio analysis also informs how BES research strategies can be designed to create opportunities for close collaboration, intersectionality of fields, and generation of human talent. Because basic energy science evolves rapidly on a global stage, identifying emerging opportunities and rebalancing priorities within the portfolio is an essential part of the mission of the Office of Science and the role of program managers.

We illustrate the power of portfolio analysis with a case study of the impact of basic science funding on battery technology and on the scientific community at large. We used publicly available data, including publications, citations, patents, awards, workforce development, and industry interactions. During the 18 years since the 2006 BRN, total U.S. funding for basic research in energy storage has been significant. Some of this funding supported activities in the Joint Center for Energy Storage Research, which produced over 750 publications (subsequently cited more than 50,000 times), more than 60 patents, and trained more than 300 researchers that ended up in academia, industry, and national laboratories. In parallel, the funding supported eight Energy Frontier Research Centers (EFRCs) focused on energy storage, which together have generated over 1,000 publications (and about 100,000 subsequent citations), in addition to training a new generation of energy researchers. These investments in fundamental energy science fostered inventions of new technology in the energy sector, as evidenced by tracking patents and intellectual property. Although China dominates current production with over 50 percent of lithium ion battery cell output, for example, the U.S. and Japan hold most of the original patents.

Workforce development is another way to gauge the impact of fundamental research. A recent report[1] shows salaries for visa holders in the U.S. battery field have increased steadily over the past few years. Moreover, between 50–120 jobs in the U.S. are created for every gigawatt hour of battery production. However, we find that students and professional electrochemistry scientists trained in the U.S. are increasingly moving abroad to work in other countries, so there is a need for incentives to retain this skilled workforce.

Another indicator of a successful portfolio is adoption and investment by industry. It is important to consider that the U.S. battery industry spans raw materials, material processing, cell components, cell manufacturing, system assembly, and recycling. Large companies in this sector have a market valuation of more than $1 billion. Moreover, the vast majority of start-up companies in this field originate in the U.S.

A summary of the findings from the report are provided here. The subcommittee recommends several strategies for successful management of research portfolios in the future:

- Continue and expand broad engagement with the research community and other constituencies to maintain and enhance technical excellence of DOE/BES science in line with its mission. Industrial engagement may help identify key knowledge gaps for DOE-relevant technologies or opportunities to develop new basic understanding.
- Balance the funding portfolio across multiple axes including research versus facilities support, single investigator versus Center or Hub funding, and support of existing program areas versus nascent fields of inquiry.
- Facilitate seamless transitions from fundamental to applied research, which may involve cross-office interactions.
- Consider the benefits of investing in and adopting tools for portfolio analysis, whether gathering raw data available online and building simple tools or building complex AI/ML learning models. Couple the use of quantitative methods with expert opinion for optimal outcomes.

[1] www.volta.foundation/battery-report, 2023

INTRODUCTION

Science and technology have become an integral part of our daily lives and now define many aspects of how society functions. In fact, today's college and university students have never experienced life without cell phones, personal computers, or the myriad of technologies that surround us. Beyond impacting our lives and work, science and technological innovation are critical economic drivers where U.S. prosperity and security are intimately linked to the pursuit and advancement of new ideas and the technologies they spawn. Technologies are typically born from scientific discoveries that can then lead to innovation that translates the discovery into something usable. Indeed, scientific research has been the basis for many key technological developments in the U.S. some of which may have emerged decades later.[2] The imperative for continued U.S. investment in scientific research was recently assessed in detail to determine the state of international competition.[3] The findings showed that due to increased international investment and the flattening of U.S. investment, the U.S. leadership position in science and technology is challenged. The criticality of U.S. investment in scientific research is apparent. Note that the findings and suggestions in this document are presented in a constructive spirit with no implication that there are significant deficiencies or gaps in current practice.

Investment by the U.S. federal government in basic and applied research has increased over the time period from 2012–2021 where a significant part of the increase since 2019 was driven by investment relevant to the COVID pandemic.[4] Notably, research costs have also increased significantly where the increases driven by inflation, supply chain challenges, and cost of living likely offset some or much of the apparent increase in research funding. As an example, the academic stipends of physics graduate students have risen by ~30% over the period from 2011–2022 (see Figure 1), and the increases are expected to accelerate because of recent inflation.[5] This serves as only an example as increases in the cost of operating facilities, new construction, hiring and retention of talent, as well as purchasing materials, all continue to rise. The resultant constraint on research growth becomes apparent.

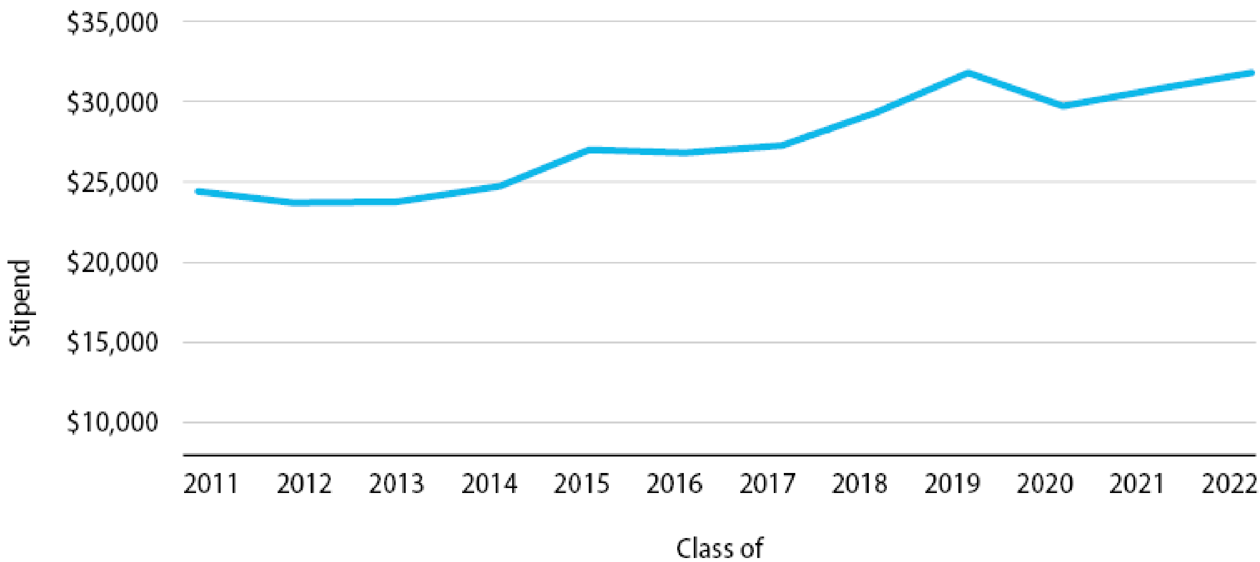
[2] *A Remarkable Return on Investment in Fundamental Research. 40 Years of Basic Energy Sciences at the Department of Energy* (U.S. Department of Energy, Office of Science, 2018), www.science.osti.gov/-/media/bes/pdf/BESat40/BES_at_40.pdf.

[3] *Can the U.S. Compete in Basic Energy Sciences? Critical Research Frontiers and Strategies.* A report by the BESAC Subcommittee on International Benchmarking ((U.S. Department of Energy, Office of Science 2021).

[4] www.gao.gov/products/gao-23-105396

[5] It is recognized that multiple fields are supported by BES, the data for physics is used as representative of the general trend.

FIGURE 1. Stipends for Graduate Student Research Assistants from 2011 to 2022



Source: American Institute of Physics, Degree Recipient Follow-up Survey

Notes: Median annual research assistant stipends for new physics bachelors pursuing graduate study in physics or astronomy. This self reported data comes from new U.S.-earned physics bachelors that were enrolled in a U.S. physics or astronomy graduate program in the winter after receiving their degree.

The tension between the need for expanded investment in research driven by global competition and increasing costs highlights the need and the timeliness to consider research investment strategies. The recent report on the status of U.S. scientific investment found that the U.S. is falling behind other nations in some critical aspects of research, including advanced facilities and instrumentation, as well as the attraction and retention of the requisite scientific talent.[2] While the report recognized the criticality of the investments and recommended further increases in spending for research, facilities, infrastructure and the associated human talent, the pace at which research investment can be expanded may prove to be a limitation. Thus, it is of critical importance to provide an assessment of research investment strategies. Costs of research are rising, international competition is strong, thus, thoughtful, and effective strategies for investment of the available research dollars are imperative. This report summarizes the findings of the subcommittee formed to address this important challenge and provide suggestions for additional strategies for assessment of research investments.

This topic has received attention from various organizations in the U.S. and internationally. Thus, the first step the BESAC subcommittee took was to assess recent reports on the topic of research portfolio assessment. It is important to consider the distinction between portfolio assessment in contrast to assessment of research programs or individual researchers where the discussion here is focused on portfolio assessment rather than the progress of any initiative. The subcommittee formed four subgroups focused on:

1. targeted outcomes for the report,

2. current practices in use by BES,
3. summary of relevant items from other portfolio assessment reports, and
4. a case study example using an array of possible methodologies.

The expanded availability and prospects for analysis tools and methods that could be employed by BES and the Office of Science and their opportunities for enhancement of current approaches are presented. Adoption of some of the approaches provides the possibility to further empower DOE/BES to better assess the balance of investments among research areas, modalities, distribution, and in order to improve the effectiveness of adjustments where appropriate.

Desired Outcomes of the Study

In the charge to the BESAC subcommittee, numerous questions are posed related to the optimum prioritization of research investments. A subgroup of the subcommittee (subgroup 1) first focused on translating this set of questions into statements of desired and achievable outcomes that the study would enable. Through a series of in-depth discussions of the questions posed in the charge letter, a set of statements characterizing the desired outcomes was developed. An effort was also made to think creatively, beyond the charge letter, about possible goals of the study. All these statements are in the constructive spirit of the charge letter concerning possible improvements and enhancements with no implication that there are significant deficiencies or gaps in current practice. Paths toward these desired outcomes are discussed in the work of the other subgroups, as some of the commentary associated with these outcome statements indicates.

Summary of Desired Outcomes

1. ***BES strengthens its investments to maintain and advance foundational scientific knowledge and international competitiveness.*** Achieving this outcome will depend in part on better metrics of success and better ways to analyze the research portfolio.
2. ***BES is nimble in investing and disinvesting in topical areas of research*.** BES has in place an effective system of Basic Research Needs (BRN) workshops and strategic planning involving the synthesis of multiple streams of input. Investing and disinvesting are not simple, reversible processes and could be enhanced by better metrics.
3. ***BES optimizes the balance in its portfolio.*** There are multiple dimensions of balance that are considered including the balance of university or national laboratory research, the balance between exploratory or mission-driven research, and that between support of research or unique national user facilities. Additionally, consideration of the funding modality supporting individual, small groups of principal investigators or Centers or Hubs. Achieving appropriate balance may be enhanced by advancements in assessment tools.
4. ***BES addresses increasing costs of research*.** Inflation, graduate student unionization, international competitiveness, and the need to improve support for mid-career scientists are among the factors

driving up research costs in a significant way. Addressing these costs may not necessarily be achieved through overall DOE budget increases, but rather through good choices in funding priorities.

5. ***BES has more effective tools for insight into evaluating basic research that is use-inspired.*** Use-inspired research can lead to new ideas about fundamental research problems. To address specifically one of the questions in the charge letter, a basic-applied research continuum is desirable. It may be useful to involve industry more extensively in strategy for some fields related to the BES mission.

6. ***BES has effective approaches for investing in and prioritizing workforce-enhancing measures relative to research, instrumentation, and facilities*.** This could mean early-stage efforts to encourage STEM (science, technology, engineering, and math) education, support of early career scientists, support of mid-career scientists, support of facilities scientists, and more, as discussed in the benchmarking study, *Can the U.S. Compete in Basic Energy Sciences?*

OPPORTUNITIES TO ENHANCE RESEARCH PORTFOLIO SELECTION

Introduction

The recommendations of the BESAC Strategy Subcommittee are made within the context of maintaining and enhancing the synergistic relationship between DOE researchers and program managers with the goal of optimizing BES' strategic research portfolio development and investment. Set against the backdrop of the rapid evolution of machine learning/ artificial intelligence and major advancements in instrumentation such as X-ray and neutron sources, researchers are encountering unprecedented opportunities for discoveries in areas ranging from new materials to sources of energy to geological processes. This exponential increase in not only scientific knowledge but also the computational capacity through which to develop and store this information creates multiple avenues for collaboration in the form of joint proposals and options for cross-funding as would naturally follow. As a result, we recommend increased emphasis on internal coordination between program managers within BES and other Office of Science (SC) divisions, for example Advanced Scientific Computing Research (ASCR), High Energy Physics (HEP), and Biological and Environmental Research (BER), as well as National Nuclear Security Administration (NNSA).

This BESAC Strategies Subcommittee has been charged with assessing and recommending opportunities to enhance or improve methods used by BES to make decisions on strategic portfolio selection. Our recommendations were developed by reviewing methods currently used by BES Program Management (PM). The subgroup's purview was research program portfolios and not individual outcomes.

Our methods included a review of current strategic practices for how BES incorporates the 20+ years of community-driven input, from the reports on Science for Discovery, to Basic Research Needs and National User Facilities, with the overarching mission of DOE, the Office of Science, and BES. The subgroup also had numerous discussions with BES leadership, National Laboratory directors, and BES-funded researchers.

To achieve the aforementioned, we recommend providing program managers with more flexibility in the means by which to communicate their vision(s) for future research with relevant and/or new communities of researchers. Keeping in mind the "two-way street" nature of communication between program managers and researchers, we realize that both parties must be open to feedback on any aspect of programs in progress. Metrics of evaluation can operate within the highest traditional standards of the DOE while still considering the overall balance of the portfolio over the dimensions discussed above. We believe that the adoption of recommendations of this nature can further empower DOE/BES to better assess the balance between mission-driven and higher-risk research undertakings while allowing and even encouraging more efficient and presumably more fruitful adjustments as necessary.

What is Working

The DOE/BES has been and remains an extremely effective organization in continuously evaluating its research portfolio. This is in no small part the result of the dedication of the senior leadership and program management who are effective and respected members of the scientific community. The ability of DOE through its Program Managers to engage with stakeholders across the breadth of the research community is critical to success and effective management of the BES portfolio. Specifically, this permits DOE/BES to effectively integrate multiple input streams and associated strategic considerations. Examples of this include the use of roundtables and workshops to generate the reports on DOE "Basic Research Needs" (BRNs) which serve to both consolidate inputs and communicate DOE/BES mission and research priorities back out to the community for consideration and execution. The BRN associated mechanisms are in many ways at the core of DOE/BES's success in managing their portfolio. In the presence of additional pressures associated with the changing environment for science, strategic management of the DOE portfolio is critical.

Spring 2023 interns work in groups to create different formulations of ice cream in the Interdisciplinary Science Building at Brookhaven National Laboratory. Source: Kevin Coughlin/Brookhaven National Laboratory

What Opportunities Exist

Broader Community Engagement

Engagement with the research community is a cornerstone of the DOE/BES success. Broadening the engagement and diversity of constituencies is key to maintaining and enhancing the technical excellence of DOE/BES science in line with its mission. DOE program management has and continues to work at broadening engagement, initiating "Office Hours" and other community outreach efforts that have low barriers to access, in addition to the more traditional roundtable and BRN development activities.

Also, DOE/BES has continued to actively steward the existing portfolio as it evolves with direct engagement with the laboratories and principal investigators. This work, with its associated demands, is an integral part of the responsibilities PMs are asked to undertake. Given the number of mechanisms to solicit input from the community, modification to these streams or additions to them must be carefully considered to ensure they do not undercut their existing effectiveness.

While caution to change must be taken, improvement is perpetually required to ensure that DOE's scientific excellence is maintained. Thus, a disciplined approach to modification of the DOE strategic planning inputs and their assessment is recommended. The committee believes that the use of big data analysis and opportunities to use machine learning to understand the impact of the portfolio should be considered. At the same time, at present the clear value proposition of these types of tools given the relatively high cost in resources means that efforts in this area should be undertaken strategically and evaluated carefully to ensure that the returns justify the investments. Other funding agencies are also considering AI/ML as a means to assess program impact. DOE/BES could consider investigating best practices being deployed elsewhere and perhaps even partner for effective deployment of such tools.

Industry Partnerships

The role of U.S. industry in both identifying topics and translating basic science insight to relevance in new or existing technologies was also extensively considered by the committee. Balancing between input from industry to identify key knowledge gaps to advance technologies within the DOE mandate and development of new basic understanding that can spark development of disruptive technology remains a challenge inherent to DOE's mission. Efforts to convene the community across constituencies should continue to be inclusive of industrial researchers to align U.S. competitive needs. While it is no small task to triangulate among BES-funded researchers, the BES mission, and industrial research needs, maintaining the equilibrium between push and pull across industrial and academic research will continue to require that input streams be maintained across these constituencies. Dialog between industrial R&D efforts and the basic science community is also integral to the identification of pathways to enable translational research efforts to bridge technological readiness levels and associated "technological valleys of death."

Partnerships With the U.S. Manufacturing Industry

The questions of what and how the scientific foundation of advanced manufacturing will be met is important for U.S. competitiveness moving forward. Stewardship of translating insight on topics spanning the DOE grand challenges into advanced technologies is an area where DOE/BES excellence is increasingly required. This requires an understanding of the existing industry practices and incentives to strategically apply basic insight into new industrial processes and ultimately products. In this context again, the push of new basic insight with the pull of incumbent technologies must be balanced as well as the management of where handoff between basic and applied can and should occur. Efforts to more effectively and efficiently transition investments across the various technology readiness levels and associated technological valleys of death requires continued stewardship and engagement with both basic and industrial research practitioners. To these ends, understanding how and why different basic R&D activities have impacted U.S. industry is required. This assignment is a broad undertaking, but key to ensuring the elements of DOE's U.S. competitiveness mission are addressed.

The inclusion of industry-based advisory boards in multi-investigator projects, as well as the inclusion of industrial researchers in advisory committees and BRN working groups, appear to be effective mechanisms currently being employed. Opportunities to capture additional data that might provide insight on impacts to industrial stakeholders based on the DOE portfolio, outside of direct engagement with DOE programs or utilization of DOE user facilities, should be considered but may present challenges.

Role of Partnerships with Publishers

The dissemination of basic R&D developments is a critical activity. The primary mode of dissemination has been peer-reviewed publications. Insight regarding the broader impacts of research publications is data which may align with the efforts of publishers to understand their audiences. Data on citations and tracking of publications and their impact is an area where DOE—as a sponsor of basic research—might be able to partner with publishers to better understand the impacts of R&D activities. The extent to which organizations that serve as publishers (like the American Physical Society or the American Chemical Society) might share data with BES is a potential opportunity to use advanced analytics to assess impact of R&D investments and the balance of the portfolio across topics and modalities (e.g. single investigator, large team projects).

Artificial Intelligence and Machine Learning

Opportunity for Agile Information Streams with AI/ML

Analysis of the research impacts and the utility of the data generated by basic R&D remains a critical objective. The extent to which advanced data analytics can be used to make these assessments is a relatively new and rapidly evolving area. There are significant opportunities for DOE/BES to examine how data that might provide insight can and should be structured to enable advanced analysis approaches. While there is significant potential in the development of ML and AI based tools, currently the expense of these capabilities are high. Given the degree to which DOE/BES is already world class at crafting a scientific portfolio, significant investments in AI/ML tools should be done judiciously considering both the possible benefits as well as the resources required. Thus, an approach that remains agile and adaptable, considering structuring of existing inputs to maximize their value while minimizing resource investments, appears prudent. This will enable DOE/BES to employ AI/ML analysis tools when upfront costs are reduced (e.g. tools become more ubiquitous), or when partnerships across agencies can reduce the opportunity cost associated with these investments.

RESEARCH ASSESSMENT: A Summary of the Existing Literature

Introduction

In response to the evolving landscape of scientific research and the increasing demand for robust assessment methodologies, subgroup 3 was entrusted with the task of synthesizing the existing literature on research assessment. The task aimed at extracting insights from a diverse array of international reports and stakeholder perspectives, with a particular focus on strategies applicable to the DOE's Basic Energy Sciences portfolio.

Over the past decade, a substantial body of literature has emerged from various international agencies and stakeholders, reflecting the growing interest and scrutiny surrounding research assessment practices. Recognizing the need to navigate this wealth of information effectively, a dedicated subgroup within the committee undertook the responsibility of reviewing and summarizing key findings from prominent reports. Notable among these are the UK Metric Tide report,[6] the working paper on Research on Research Institute (RoRI),[7] the Strategic Plan of the NIH Office of Portfolio Analysis (OPA),[8] the National Academy report on the foundations for a vital research community at NASA,[9] the San Francisco declaration on research assessment (DORA)[10], and the Leiden Manifesto.[11]

Assessment of these documents revealed significant common threads, that could be consolidated into three major subsections: i) publications, patents, and other numerical metrics, ii) methodologies including artificial intelligence/machine learning (AI/ML) tools for portfolio assessment, and iii) expert input into planning of research directions. Each subsection below corresponds to one of these specific thematic areas, with references to the individual reports for detailed content.

Central to our approach is a focus on research portfolio analysis and not single Principal Investigator (PI)

6 www.ukri.org/publications/review-of-metrics-in-research-assessment-and-management

7 www.researchonresearch.org

8 www.dpcpsi.nih.gov/opa/strategicplan

9 www.dpcpsi.nih.gov/opa/strategicplan

10 www.sfdora.org

11 www.leidenmanifesto.org

assessment. While acknowledging the richness of literature addressing single PI assessment, our report draws inspiration from these sources to extract insights applicable to broader portfolio evaluations within the context of DOE/BES. These considerations are reflected in our recommendations and conclusions.

An overarching concern that permeates the discourse on research assessment is the role of diversity and inclusion. There are inherent biases present in both quantitative metrics and qualitative judgments, underscoring the importance of fostering diversity in backgrounds and expertise among those involved in shaping assessment strategies. Ensuring broader representation and perspectives are the best countermeasures to mitigate the risks posed by biased assessments and to foster a more equitable research environment within the DOE/BES community.

Findings

Quantitative Metrics

The assessment of research quality and impact is a critical aspect and the use of publication metrics plays a pivotal role in this process, providing quantitative data to gauge the influence and reach of research outputs. However, a nuanced and balanced approach is essential, as relying solely on quantitative metrics can lead to unintended consequences and distortions in research assessment.

An important benefit of quantitative objective metrics is that they allow responsible research evaluation and mitigate biases within peer review processes (see Leiden Manifesto, Hicks *et al.*, 2015). At the same time, many of the reports (Leiden Manifesto, UK metric tide, DORA) emphasize that decision-making should not be exclusively driven by numerical data. Instead, the informed judgment of domain experts should be coupled with these metrics to avoid some pitfalls in research assessment (Wilsdon *et al.*, 2015). As discussed in the UK Metric Tide report, in fact, some quantitative indicators, such as journal impact factors and citation counts, can be manipulated and may not capture essential aspects of research, such as inclusivity and research culture. Another aspect is related to the importance of normalizing metrics by field, as there can be significant variations in impact factors, publication and citation rates, and other indicators across different disciplines. Here a possible solution is offered by the NIH report which introduces the Relative Citation Ratio, a metric that accounts for variations in citation rates across different fields (Hutchins *et al.*, 2016). This innovation aims to make research assessment more equitable and field-specific. Regardless, regular scrutiny, evaluation, and adaptation of chosen metrics are vital to ensure their relevance and fairness.

Generally, it seems good practice to combine as many indicators as possible to provide a more comprehensive assessment, while avoiding the illusion of false precision. As emphasized in the RoRI report there is a need for a holistic and adaptive approach to research assessment. Relying solely on narrow criteria can lead to distortions and ethical challenges. Embracing open access, data sharing, diversity, and aspects such as knowledge transfer and commercialization of research products reflects a progressive evolution in the way research is evaluated and valued. In this regard, it is in there noted that one of the largest jumps in future focus is the translation of research findings (via knowledge transfer and commercialization) to societal benefit. Currently only 2% of the funding agencies surveyed use a metric focused on this translational aspect, whereas an additional 10% indicate that they would use such a metric in the future (5x increase) (Moher *et al.*, 2016 Fig. 3, p. 33).

It is important to consider how the assessment metrics can have either a positive or negative effect on achieving programmatic Diversity, Equity, and Inclusion (DEI) goals. As one example, narrow indicators of research productivity can lead to systemic biases, especially for efforts that lie at the boundary between basic and applied research, and they can also limit the diversity of proposed research missions and limit flexibility in cross-cutting activities. Concurrently with the development of appropriate metrics, it is critical that training resources are available at all levels of the assessment and review process to ensure that all parties understand and fairly evaluate based on the prescribed assessment approach.

Overall, the reports collectively emphasize the need for a balanced and comprehensive approach to research assessment. While publication metrics are valuable tools, they should be viewed as one component of a multifaceted evaluation process. Qualitative evidence, expert judgment, and consideration of the specific context within each academic field should also play a significant role in assessing research quality and impact. Additionally, ongoing scrutiny and adaptation of assessment practices are essential to ensure that they align with the evolving landscape of research and academia.

Methodologies and AI/ML Tools in Research Assessment

The research assessment tools can be applied at the portfolio level or at the individual researcher/project/output level. Publications, citations, and other metrics discussed above typically focus at the individual researcher or portfolio level. OPA has developed some new tools or metrics to analyze the impact that an individual publication has on the scientific field or on specific desired outcomes. In addition to the Relative Citation Ratio discussed earlier, that provides a field-normalized article-level metric of influence, OPA has developed an AI/ML tool to predict the likelihood that a given publication has translational potential and will impact clinical research.

In addition to focusing on the impact of individual publications, OPA is developing and disseminating a multifaceted assessment approach to analyze entire portfolios of funded research projects with approaches such as use of AI/ML, graph theory, and natural language processing. Portfolio analysis can potentially be used by decision makers to assess past impact and also predict the likelihood of desired outcomes resulting from the portfolio of funded projects. OPA is using these approaches to cluster topics within a portfolio to identify overlaps (see Figure 2) within NIH and even across agencies, and to also help identify emerging areas. In addition, OPA is pursuing the opportunity to improve decision making by finding gaps in the NIH portfolio and identifying missed opportunities where the investigator(s) succeeded as biomedical researchers despite not receiving NIH funding. OPA is focused on the emerging field called metascience that helps understand how discoveries arise, and the factors that propel scientific advances.[12]

[12]. For example the NIH IQRST framework (adapted from Fig. 6 in the NIH report) for evaluating productivity relies on: I=Influence (Relative Citation Ratio); Q=Qualitative Human Judgement; R= Rigor/Reproducibility of research; S=Sharing of scientific data/resources; T=Translation/Tech Transfer. Therefore, to assess the ability to result in desired NIH outcomes, OPA is also developing methods to measure scientific rigor and reproducibility and effective data/resource sharing, in addition to assess the translational potential (knowledge transfer and commercialization) of the research findings.

When such new tools and approaches utilize large data sets, a broad range of trustworthy and validated data sources from a variety of document types are needed for such an approach to lead to meaningful inferences. And while these are powerful tools, they can potentially lack transparency, unless the underlying code and data sets are publicly available.

Multiple reports have advocated the importance of the use of simple *and* transparent tools, both for data collection and for the creation of indicators for assessment, to avoid "black-box" evaluation constructs (Leiden, UK Metric tide). Transparency and openness in the research assessment processes is key, and clear criteria and methodologies should be used when metrics are employed. Those being evaluated should have the opportunity to ensure that the data being used is trustworthy and accurate. Publishers should require digital author iDs for manuscript submissions and digital object identifiers (DOIs) should cover all research outputs. To help address some of these potential issues, future strategic directions that OPA plans to address include new processes to distinguish homonymous authors, to accurately separate the contributions to the research and attribute the research products with multiple funders, and to characterize collaborative research using better approaches.

Expert Inputs

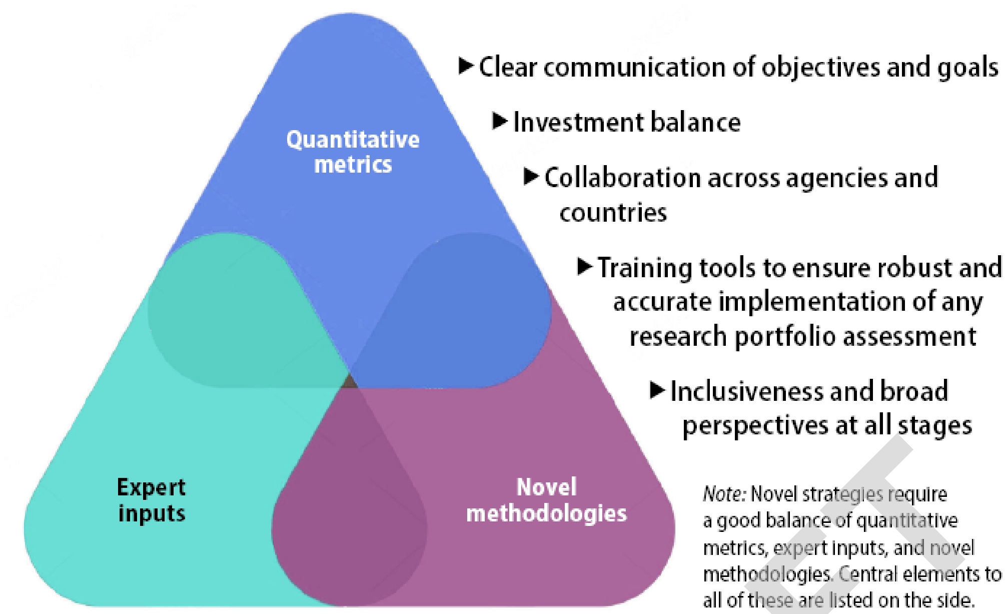
Expert panels play a key role in the assessment of research quality and impact within the academic and scientific community. The use of publication metrics, while essential, must be complemented by expert judgment to ensure a balanced and comprehensive evaluation process. Several influential reports outline best practices and provide key recommendations for expert panels engaged in research assessment (Leiden Manifesto, the UK Metric Tide report, the NIH report, the RoRI report, and the DORA document).

Expert panels should be composed of individuals with deep domain knowledge and are essential in addressing the limitations inherent in relying only on publication metrics.

The composition of the panels should moreover reflect broader interest and all the inclusion criteria to maximize the different point of views and ensure that there are no holes in the research assessment. The experts should make attempts to provide an informed judgment that complements quantitative data, ensuring a more comprehensive and fair evaluation of research contributions (i.e. Combining Quantitative Metrics with Expert Judgment as discussed in the Leiden Manifesto).

For panels covering research in multiple areas, there is also the need for field-specific normalization recognizing substantial variations in impact factors, publication rates, and citation rates across different academic disciplines. As recommended in the UK Metric Tide report, it is imperative to normalize metrics by field to ensure a fair and equitable assessment. Expert panels should consider the adoption of such field-specific metrics to enhance the precision of assessments as put forward in the RoRI report. Furthermore, various dimensions of research should be evaluated including basic and applied aspects, open access publications, data curation, diversity and inclusivity, and knowledge transfer and commercialization. Considerations of diversity, equity, and inclusion in the research assessment process can lead to overall positive momentum towards achieving the scientific, cultural, and demographic goals of the overall program. These factors should be considered at all stages of the research evaluation process, ranging from community input into research avenues to detailed assessments at the proposal, portfolio, and programmatic levels. For example, the composition of panels that generate decadal surveys and guiding research reports should be scientifically robust, and culturally and demographically diverse to foster innovative idea generation and to reflect a broad spectrum of viewpoints.

FIGURE 1. **Novel Strategies for Research Assessment**



Among the reports surveyed, self-evaluation was only strongly emphasized in the Netherlands report, although input from the researcher during assessment is encouraged in the UK metric tide report. In the case of the Netherlands report, quantifiable metrics are self-reported alongside qualitative metrics. This allows for qualitative analysis distinct from more commonly utilized metrics that consider the number of highly cited papers from a given author (H-index) or journal (impact factors). However, including a self-assessment may be more time-intensive for the principal investigators and may present challenges in direct (apples-to-apples) comparisons between PIs during the committee assessment.

Self-assessment provides an opportunity for principal investigators to assess the alignment of their own research with larger program incentives and targets. Thus, creating a self-assessment may have the added benefit of researchers gaining a better understanding of the program, driving engagement with the program and personal ownership to achieve program objectives.

Recommendations

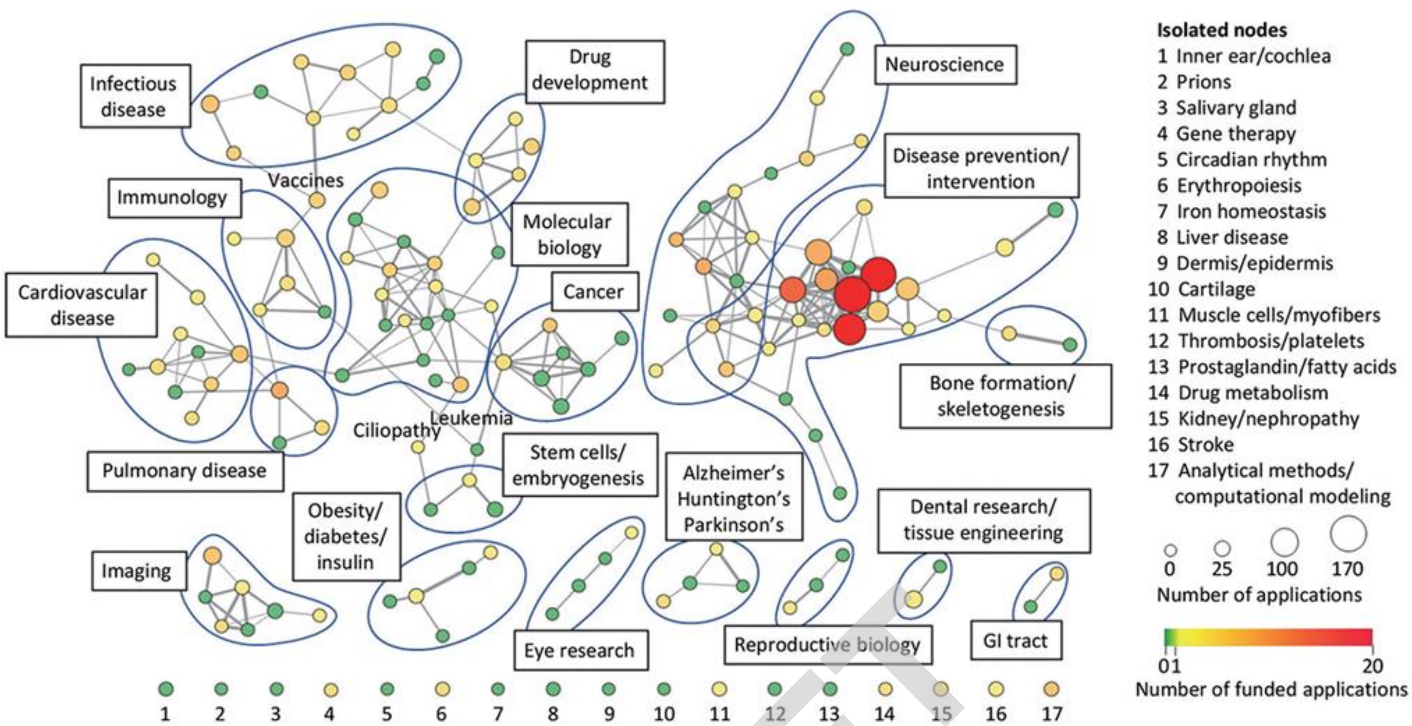
Based on the various reports, some recommendations for analyzing a portfolio of projects (such as a scientific program, a specific funding mechanism, or Basic Energy Sciences as a whole), are summarized here.

The desired goals of the portfolio need to be clear, well-defined, and assessable, and should be communicated internally and externally, to facilitate assessment of impact, as well as to engage policy makers and the general public, while fostering inclusivity. Research portfolios should be assessed for investment balance (for example striking a balance between national laboratory vs. academia, single vs. multi investigator, investigator-initiated vs. specific targeted areas) to investigate the impact of different funding distribution mechanisms on achieving the desired stated goals.

A balance of qualitative with quantitative metrics should be used for evaluation, although the methods for collecting these can vary. Publications, citation counts, and patents are examples of quantitative metrics that can and should be made available and used to inform expert panels. Careful selection of targeted metrics for different programs and different fields or communities (e.g. early career investigators as opposed to large interdisciplinary team projects, or differences based on different fields of research) is important. Key data also can be gleaned from methods such as tracking of funding acknowledgements outside of publications, to assess translation impact of basic science research (disclosures, patent applications, licensing, and workforce development among others). Positive and negative (intended and unintended) consequences of assessment policies and metrics on achieving stated goals should be considered. Finally, indicators should be regularly scrutinized and updated with modern tools and consistency with the stated goals.

New tools (AI/ML/language processing) are one option to evaluate the portfolios and their impact on achieving the stated goals. New tools should be evaluated for appropriate application to BES, and multiple metrics need to be integrated using transparent and trustworthy data sets and approaches to obtain a holistic assessment. Consideration of implementation cost is a factor in choosing additional assessment approaches, but portfolio analysis is possible using currently available tools (subgroup 4 provides an example). Collaboration across agencies for common tools and assessment strategies can mitigate the cost of implementation and also help with the identification of emerging initiatives and potential overlap with different branches of DOE or other funding agencies, leading to joint support of cross-cutting initiatives.

FIGURE 2. Distribution of Applications and Awards for African American/Black Scientists Across Topics in the NIH Portfolio



Source: Hoppe TA , Litovitz A , Willis KA , et al. Topic choice contributes to the lower rate of NIH awards to African-American/Black scientists. *Sci Adv.* 2019; 5(10):eaaw7238. https://doi.org/10.1126/sciadv.aaw7238.

Note: Each node in the network represents a topic cluster, and related topic clusters are grouped inside blue borders and labeled (rectangles). Node size correlates with the number of applications and nodes are heat-mapped by the number of funded applications from African American/Black scientists in each cluster.

Training tools are necessary to ensure robust and accurate implementation of any research portfolio assessment approaches that also consider explicit and implicit bias. When appropriate, expert pools should be assembled at all stages of the portfolio ideation and research assessment process, keeping in mind diversity (scientific, cultural, etc.) and inclusiveness of different perspectives.

PORTFOLIO ANALYSIS: A Case Study

Introduction

Basic energy science research requires substantial and sustained investments of time, funding, and human talent to realize its full potential and value to society at large. Allocation of resources to support BES research reflects shared interests among researchers, stakeholders, and stewards. The DOE Office of Science organizes and engages these communities in regular workshops and roundtables, providing transparency by establishing priority research directions and opportunities. Subsequent to these activities, funding opportunities are announced, and portfolios of projects are assembled with contributions from single-investigators, small teams, energy frontier and energy earthshot research centers, and hubs. In this way, a diversity of approaches and perspectives can be pursued in parallel while also remaining unique in their focus to avoid redundancy.

As portfolios within BES sub-disciplines mature, it is useful to verify that scientific foundations have been laid that will sustain growth of new science fields and disciplines (such as, neuromorphic computing, quantum materials, and quantum information science) and assess whether existing research programs continue to advance scientific knowledge and leadership with demonstrable impact.

Portfolio analysis therefore emerges as an important tool for the Office of Science, as described in the previous section. It helps ensure resources are being allocated efficiently and effectively. It can also identify underperforming areas that may need more support or areas where resources could be better utilized elsewhere. Strategic planning for current programs and their sustainable growth must be balanced with allocations for emerging opportunities and initiatives of strategic and scientific importance. Portfolio analysis also informs how BES research strategies can be designed to create opportunities for close collaboration, intersectionality of fields and generation of human talent, bringing together complementary know-how, research capabilities, and leverageable institutional and national lab resources. Structuring communication within teams is critical for establishing trusted relationships with the Office of Science and other stakeholders regarding the objectives and achievements of programs in the portfolio.

Because basic energy science rapidly evolves on a global stage, identifying emerging opportunities and rebalancing priorities within the portfolio is an essential part of the mission of Office of Science and the role of program managers. As part of their responsibilities, the Office of Science Program Managers identify new fields of research with the potential for disruption that may be nascent but are primed for future BES investments. Program managers undertake risk assessments of emerging opportunities for a complementary understanding of what would happen if the U.S. was left behind resulting from a lack of sustained investment. Program Managers pivot or refocus investments as necessary in order to keep BES programs adaptable and responsive to a broad spectrum of changes in the field.

This knowledge requires articulation of key performance indices for the creation and dissemination of scientific knowledge, scientific leadership and stewardship, enabling infrastructure, human talent development, and community engagement. Thus, quantitative assessments of these key performance indices become essential for monitoring the impacts of projects and programs sponsored by the Office of Science. Articulating specific objectives to track longitudinally establishes a system of shared values between stakeholders and the Office of Science. Office of Science has an interest in streamlining processes for monitoring and tracking progress for these key performance indices. A growing number of digital tools, as described in the previous section, are available to deliver some information in a data-driven manner to reduce the administrative and resource burden of reporting these metrics, which are considered important to maintain high scientific and ethical standards.

Description of the Methods

In a sample portfolio analysis, subgroup 4 collected data on what we consider to be the most significant indicators for measuring the impact of fundamental science research. We relied on publicly available data via Web of Science, Google Scholar, as well as public reports from various consortia and non-profit foundations. As a test case, we sought to provide a comprehensive and data-driven case study of the impact of basic science funding on battery technology and the scientific community at large. The data set included publications, citations, patents, awards, workforce development, and industry interactions. We also collected and compared the funding levels of major energy storage research centers and consortia with similar activities in U.S., Europe, and Asia. This analysis should catalyze in-depth conversations on the impact of fundamental science in battery materials and technologies and their trajectory for the future.

There are important timelines we marked for the background and context of the data and method:

1. The lithium-ion battery was commercialized in 1992 by Japanese industry, primarily for portable electronics such as cell phones;
2. The first Basic Research Needs (BRN) Workshop Report on Energy Storage by Basic Energy Sciences was prepared in 2006, with a second prepared in 2016;
3. The Nobel Prize in Chemistry was awarded to the inventors of lithium ion batteries in 2019; and
4. Global production of lithium ion batteries reached 1 TWh/year in 2023.

In the U.S., the total funding for basic science research in energy storage has been significant. Some of this funding supported activities in the Joint Center for Energy Storage Research (JCESR) and eight Energy Frontier Research Centers. Founded in 2012, JCESR was one of the DOE's Energy Innovation Hubs seeking to advance promising areas of energy storage science and engineering from the earliest stages of research to the point of commercialization. JCESR alone produced over 750 publications (>50,000 citations), over 60 active patents, and more than 300 alumni spread over in academia, industry, and national laboratories. Three startups spun out of JCESR activities; combined, they have attracted over a quarter billion dollars of private investment and (at the time of this report) are building MWh-scale energy storage systems for electric vehicles and grid storage. In parallel, the eight energy storage-focused Energy Frontier Research

Centers (EFRC) combined have also generated over 1,000 publications (~100,000 citations) and acted as a pipeline to develop the next generation workforce in this field. In addition to the Hub and EFRCs, BES has supported battery research via its core program in national laboratories and universities. As groundbreaking research has matured to higher Technology Readiness Level and Manufacturing Readiness Level, additional funding from DOE's applied research programs has followed. Noteworthy investments have been made by the DOE Office of Energy Efficiency and Renewable Energy Vehicle Technology Office through several multi-institutional consortia comprising researchers from national laboratories, industry and universities to make progress in fields relevant to transportation batteries.

We also surveyed funding for energy storage science in China, Japan, South Korea, Germany, and the United Kingdom for their major R&D expenses. Across Asia (China, Japan, and South Korea), funding for energy storage science has been steady over the last two decades, yet increasingly augmented by substantial industrial-scale R&D support from the private sector. The UK launched the Faraday Institution, while Germany has launched similar efforts focusing more on battery technologies beyond lithium ion. The approach in the UK has been to break down traditional barriers between basic research, technology development, and commercialization. For example, the Faraday Institution encompasses energy storage research and skills development for human talent, but also in-depth market analysis and support for early-stage commercialization through partnerships. This approach seeks to bring together research scientists and industry partners on projects with commercial potential that will reduce battery cost, weight, and volume; improve performance and reliability; and develop whole-life strategies, including recycling and reuse. Similar activities in the U.S. are often funded separately by different offices within the DOE providing opportunity for cross-office coordination.

Results

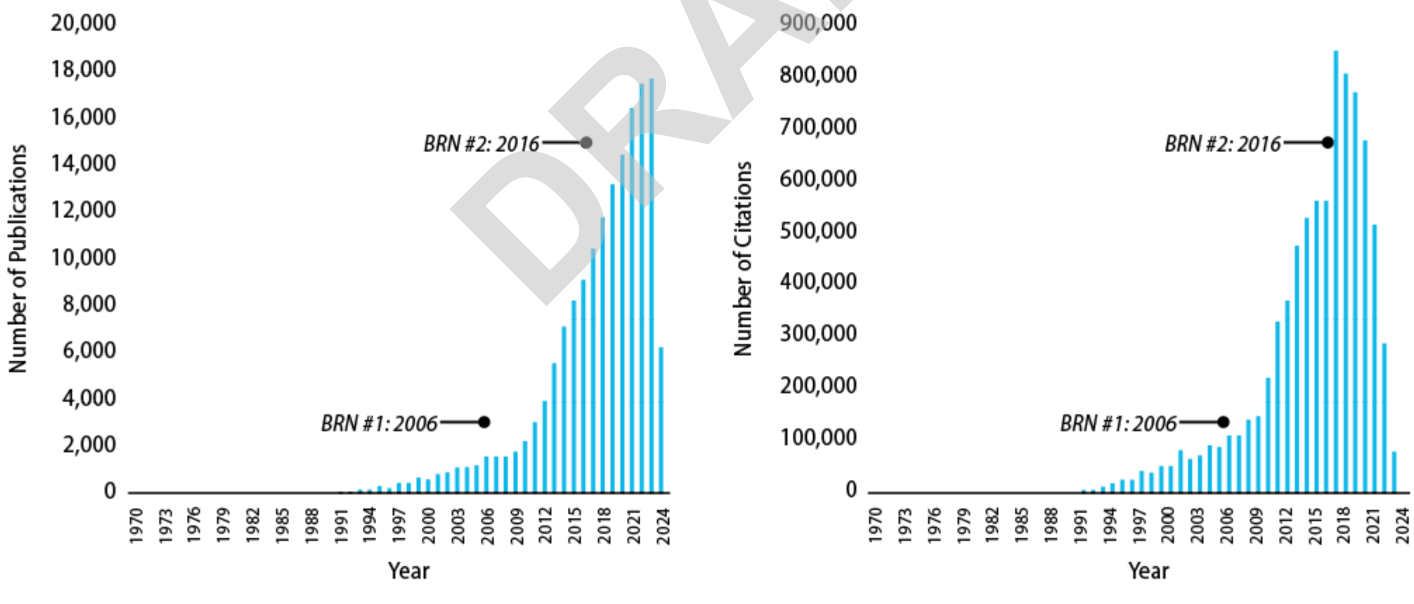
Based on the review of various reports and literature on research assessment, this committee recommends that portfolio management should incorporate multiple dimensions of input and should not rely solely on numerical metrics, such as the number of publications, citations, or patents. Our recommendation is also to use a holistic approach that involves both quantitative and qualitative measures. This inclusive approach requires scientific field-specific normalization (to account for observed differences in citation counts among different research fields) of these metrics, as well as looking at other factors, such as awards, fellowships, workforce development activities and community outreach, technology transfer successes, and other important interactions with industry.

The example of batteries is a success story, involving investments from the Office of Science, the DOE's Vehicle Technology Office, and other new DOE programs including the Advanced Research Project Agency-Energy. A second Basic Research Needs Workshop was organized to update the science questions in the field in 2017 for next generation electric energy storage needs. A search in Web of Science with key words "lithium battery" and "lithium-ion batteries" showed the exponential growth in publications and citations with an onset in the timeframe of the workshop (see Figure 1.) Cell phones had already adopted lithium-ion battery technology in the late 1990s, but the dramatic increase in publications coincides with the first basic research needs report on the topic in 2006. Similarly, battery electric vehicle adoption took place in the early 2010s and its rapid acceleration in 2020s further showcases the timeliness and relevance of the Basic Research Needs Workshop Reports.

Publications and Citations

Exponential growth in publications and patents in a topic within a field in science can be an indicator of the field's success in translating the associated technology. Early signs of that growth trajectory is, however, harder to discern. The process of invigorating a field that Office of Science has done with Basic Research Needs cross-disciplinary workshops and more field-specific roundtables has had a substantial effect in the growth of a field, evidenced in the 2006 report on electrical energy storage to this exponential growth in publications. Still, the number of citations can also inform us of broader changes in research directions. In keeping with the same test-case, by searching for both number of publications and number of citations using key words "lithium battery" and "lithium-ion battery," shown in the following plot, the data demonstrates how fast this growth took place. It is also interesting to note that the citations reached a maximum in 2017 and have been gradually declining. This is most likely due to full commercialization of this technology and the fact that researchers are now working on alternative battery chemistries, such as sodium, magnesium, and aluminum, in addition to silicon and sulfur chemistry in liquid- and solid-state batteries. We also note that evaluation of citations is context-dependent and can drop off for older publications. In applying these longitudinal analyses of publications and citations for portfolio management purposes, we encourage analysts not to use exact numbers, but to identify trends and indicators of a mature field, such as those are captured in Figure 1.

FIGURE 1. Publications and Citations on Lithium and Lithium-Ion Batteries



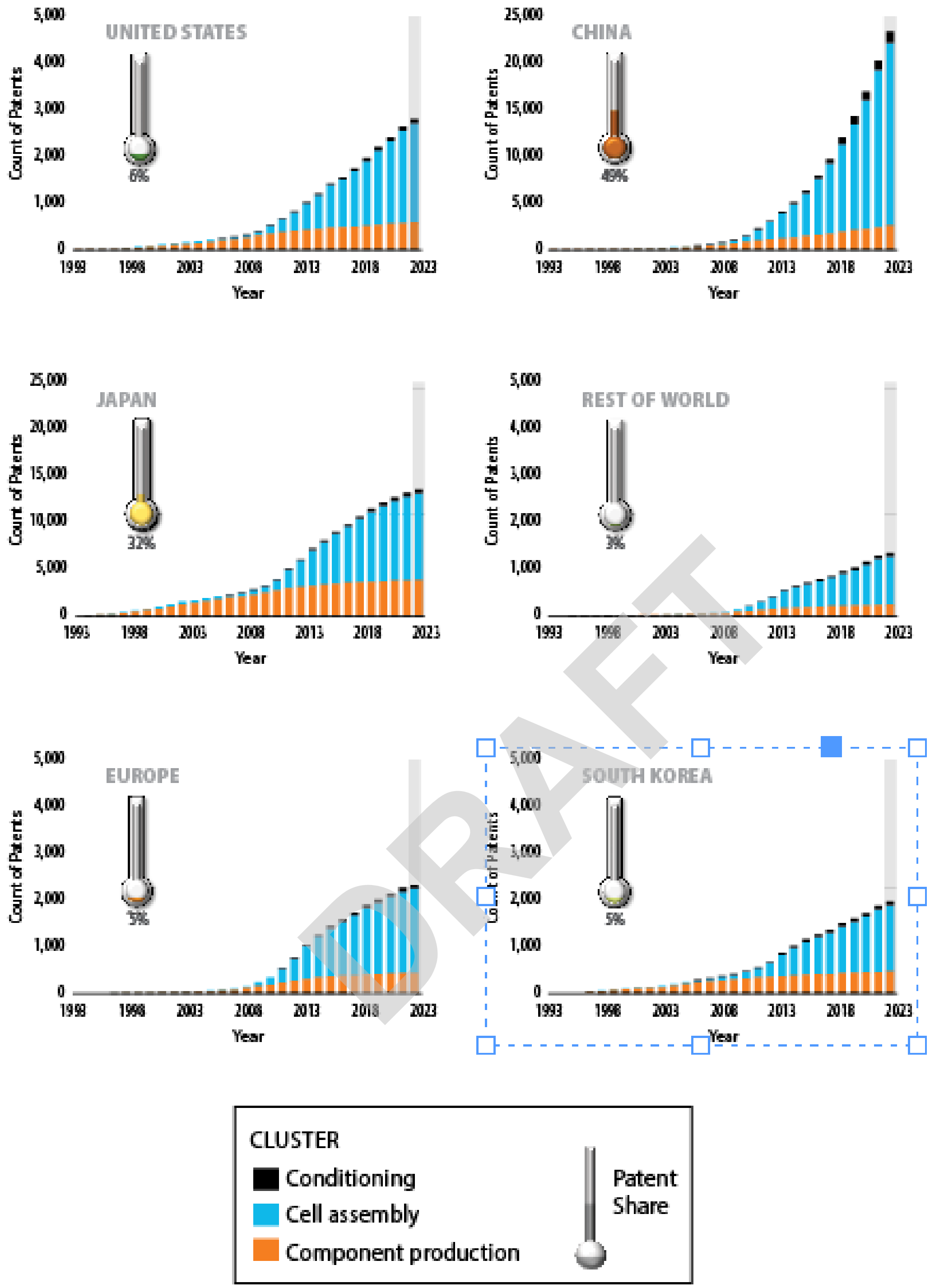
Source: Web of Science

Note: Total number of publications (left) and citations (right) is shown as a function of time since 1970s.

Patents and Utilizations

The BES research mission can be described as providing a knowledge base to help understand, predict, and ultimately control the natural world and to serve as an agent of change in achieving the vision of a secure and sustainable energy future. Given its mission of supporting fundamental science, BES in effect fosters inventions of new technology in the energy sector. As a result, tracking inventions via patents and other Intellectual Property (IP) provides yet another dimension in portfolio analysis. In the lithium ion battery sector, while China dominates in the total number (over 50%) of lithium ion battery cell production, the U.S. and Japan still hold most of the original patents and have a strong influence on other patent families. Similar to Web of Science, these data are also publicly available using Google Patent, World Intellectual Property Organization, and the U.S. Patent and Trademark office. An in-depth analysis of international patenting trends has been published by Gritemeier and Lux in 2024 (see Figure 2), where they point out that China surpassed Japan in total patent count in 2018 but Japan served as a pioneer regarding battery technology and had the largest number of granted patents from 1993 onwards.

FIGURE 2. Cumulative Patents by Region



Source: Greitemeier, Tim and Lux, Simon, *The Intellectual Property Enabling Gigafactory Battery Cell Production: An In-Depth Analysis of International Patenting Trends*

Available at SSRN: **https://ssrn.com/abstract=4766791** *or* **http://dx.doi.org/10.2139/ssrn.4766791**

Note: Patents were divided by three clusters: component production (I), cell assembly (II) and conditioning (III). Patent shares of each region in 2021 and Eigenvector centralities of each region across value chain.

The United States' global economic and scientific dominance is reflected in its patent portfolio, which emerged as the most impactful across all regions in the world. The U.S. is especially notable due to its significant influence throughout the value chain, reflected by the superior interconnectivity of patents from materials to process, and from cell to pack design. Despite the low percentage of the patents from the U.S., those patents are the more substantial and disruptive ones for the field.[13]

Workforce Development

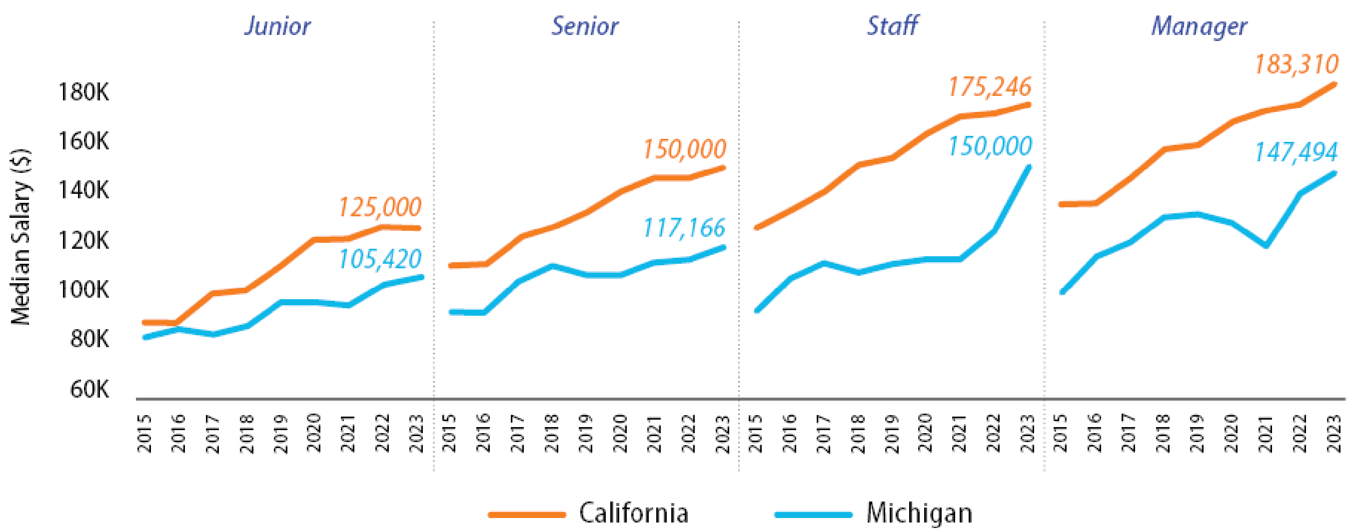
In the last century, the U.S. has dominated in the scientific arena, in a large part due to its investment in science and technology, initially from curiosity-driven fundamental science to more applied aspects and the integration of transferrable knowledge from adjacent fields, particularly chemical and materials refining and manufacturing as well as engineering know-how, such as the design and precision tooling of custom-purposed equipment used in giga factories to maintain high yields and thereby economic viability for battery production in the U.S. As a result, not only did U.S. universities produce a vibrant scientific workforce, it also attracted the best in the world to strive to come and get trained in U.S. universities and ultimately become a part of the highly productive workforce in the country. In the recent report[14] published by non-profit organization Volta Foundation, salaries for H1B visa holders in the U.S. battery field have steadily increased over the past few years (see Figure 3). More strikingly, according to both academic research and the McKinsey report,[15] between 50–120 jobs are created for every GWh of battery production.

[13] Weltklassepatente in Zukunftstechnologien, Bertelsmann Stiftung (2020). A report on World Class Patents in Cutting-Edge Technologies.

[14] www.volta.foundation/battery-report, 2023

[15] Ibid.

FIGURE 3. **Median Salary for H1B Visa Applications in Battery Manufacturing Jobs**



Source: Volta Foundation, *2023 Battery Report*

This winning recipe is now being followed by many other countries in the world, and the U.S. is no longer the only destination attracting the best human talent. Anecdotally, we found that some students and professional electrochemistry scientists trained in the U.S. are now going to other countries to lead efforts abroad. There is a need for incentives to retain this workforce. We find that BES may play an important role in future workforce development and inclusivity, where researchers from around the globe can collaborate freely and exchange ideas that lead to breakthroughs. This role is a notable counterpoint to the increasing number of restrictions regarding who can participate in research and development activities within the applied offices of DOE, due to concerns regarding unmanaged flows of information in emerging energy science and technologies of strategic interest to the U.S. It remains unclear what the long term impact of these changes will be on the scientific community and global impact.

Industry Interactions

Another indicator of a successful portfolio is adoption and investment by industry. For a nascent energy technology, early adopters are generally new companies and startups, as more mature industry players are often risk averse for new technology because they are focused on keeping pace with customer demands for their products and maintaining supply chains and quality standards to ensure high yields and therefore profit. In extreme cases, current industry may advocate against technologies that disrupt their business model. For example, in the early 2000s, responding to the California Air Resources Board (CARB) zero-emissions mandate, automakers had produced >5000 vehicles for lease. In response, however, the oil industry pressured CARB to rescind the mandate through a combination of lobbying and lawsuits. During this time, the oil and gas industry also pushed for hydrogen-powered vehicles, since they were also hydrogen producers and would therefore not be left behind in the transition. Thus, the advancement of disruptive energy technologies is not always dependent on purely technical factors.

However, in the time between the early 2000s and today, with substantial improvements in the technology enabled in part by BES funding, the battery electric vehicles today are on a much stronger foundation and trajectory than they had been previously.

With respect to creating and sustaining value from BES investments in energy storage, it is important to consider that the U.S. battery industry currently spans raw materials, materials processing, cell components, cell manufacturing, system assembly, and recycling. This alone has >$1B market valuation for large companies (public and private) along with ~$30–100M valuation for small startups. The vast majority of the start-up companies in this field originate from the U.S., thanks to its entrepreneurship core values and increasing support and stewardship for entrepreneurs from universities and national labs. Yet, these companies are still exploring business models for turning a profit. For example, Tesla's business model was to become an automotive original equipment manufacturer (OEM), rather than a battery supplier to current automotive OEMs. However, more recently, startups have pursued alternatives, including licensing models. Still others are integrating themselves as component suppliers in the supply chain for domestic battery production with support from the Bipartisan Infrastructure Law. In this way, pathways to value creation for long term benefit to the U.S. manufacturing economy continue to inspire creativity. The portfolio of technologies from BES aimed at different sectors of the industry also allows business models to be tested and refined.

While individual market valuations and collective economic prosperity are measures of success in technology translation to products, for portfolio management, it is important to identify earlier on—during the fundamental research stage—what might ultimately be its impact on society. The success of bringing batteries from fundamental science research to a widely adopted technology is a result of close collaboration of BES with more applied research agencies. Often technical challenges faced in applied fields can identify gaps in fundamental understanding in a phenomena so a feedback loop is needed between these two for successful hand-offs. Watching early entries in industry and investment such as SONY in the case of lithium ion batteries, or Microsoft, Google, Amazon, IBM, etc. in the case of Quantum Information Systems are often indicators of progress in a field. If possible, exploring opportunities jointly with industry to identify the fundamental gaps in science could benefit the choice of topics for research. Likewise, exploring opportunities for technology translation could benefit from engaging business school programs around the U.S. as well as recent DOE programs, such as Energy I-Corps and the Lab-embedded Entrepreneurship Program (LEEP) fellows.

International Benchmarking

Tracking investment by other governments in basic science and assessing the impacts of intellectual output from those investments are also critical to maintaining competitiveness on a global stage. This information may not be publicly available or, in some cases, sensitive. To the extent possible, building close relationships with funding agencies and program managers abroad would lower perceived barriers to communication, create a more informed perspective, and even provide insights for strengthening international cooperation. In general, the research community in a topical area can also help to acquire this information. For example, the UK Faraday Institution has a similar scale of scientific investment in next generation battery technology as the U.S. Energy Innovation Hub JCESR. Japan's green technology excellence program, funded by the Japan Science and Technology Agency, involves over 120 scientists from

50 institutions in Japan (~US$100M for 5 years), focusing on topics such as solid state batteries (sulfides and oxides), sodium batteries, lithium-sulfur batteries, as well the digitization and characterization of these emerging new battery chemistries.

Implications and Recommendations

1. **Balancing the funding portfolio:** Divestment in mature topics should be carried out in a careful manner that reflects future potential for impact, where leading indicators are often declines in total citations, an increasingly saturated IP landscape, and the pervasiveness of niche scientific discoveries in a given field or topic. Divestment could be accompanied by investment in new emerging topics, including those utilizing existing capabilities and infrastructure initially built for other purposes to minimize the impact on researchers and institutions. For instance, the immense scale of long duration energy storage, materials requirements, and system level demands are completely different from those needs in the mobility sector. The scientific community should consider and plan the BRN workshop and assess the gaps in fundamental understanding of matters for this mission driven research.
2. **Creating a seamless transition from fundamental to applied research:** Emerging technology is hard to predict, when the concepts are still in the idea and proof-of-concept stages. Basic Sciences are the starting point, and very often these earlier understandings are absolutely key to make progress in any field. Curiosity-driven science can also lead to discovery by serendipity, and often can start a whole new field of science and applications. However, curiosity-driven science is underfunded in the U.S., likely due to strained resources. Establishing mechanisms ensuring a seamless transition from fundamental science to use-inspired science can be considered as a continuum and provides opportunity for researchers to collaborate towards a common goal. The Office of Science recently started recently started a program called ACCELERATE for innovations in emerging technology to bridge the so-called "valley of death." This is a program that will highlight how fundamental science, funded by the public, is critical for emerging technology. Simultaneously, it is also critical to continue the core programs within BES, which are truly the seat of discovery of new phenomenon that oftentimes is not use-inspired but yields immensely important knowledge for the understanding of the nature of materials around us.
3. **Investing in tools for analysis:** Use of some very simple tools can go a long way in identifying the trends in how a science field is progressing. While avoiding dependence on any singular metric, trends can help program managers make informed decisions on topics for investment. We used Web of Science keywords to look at publications and citations. During this data collection, we also found that the user interface provided by Thomson Reuters is somewhat limited. However, the raw data is available for download and relatively simple python scripts allowed us to automate the download and analysis of the data beyond what is currently offered in the web portal. We also found additional useful tools such as VOSviewer, which was developed by Leiden University and is a freely downloadable tool that works with data from Web of Science. Other agencies such as National Institute of Health, have done extensive analysis for portfolio management and have invested resources, such as building artificial intelligence/machine learning models. Some agencies, such as NIH and Office of Naval Research, have separate offices dedicated for such activities. The potential for collaboration with these agencies could be considered. In our efforts to look into some of this digital infrastructure, we found that some simple

tools can be developed, possibly with community input and without large investments, that may benefit BES researchers and program managers alike in their shared interest in stewarding scientific discoveries and breakthroughs to their most effective ends.

OUT OF THE BOX APPROACHES

This report presents an overview of the objectives and benefits of strategies for evaluating research investments, opportunities for adoption by DOE/BES, assessment of prior literature on the topic, and a case study example that can be used as a model for future analyses. These illustrate multiple approaches to assess the strength and possible trajectory of a research portfolio. More challenging, however, is projecting nascent or emerging areas of inquiry that may prove important in the future.

To address this issue, we offer "Out of the Box" ideas, based on our discussions, that could be considered to gain insight into new arenas of science. We offer these not as specific recommendations, but rather as thought-starters of new places to look for information on emerging topical areas. We suggest these topics without full knowledge of all the activities that the program managers pursue, so some may duplicate activities already in place, but knowing that BES can evaluate and select suggestions that prove appropriate.

- ❑ Conduct intermittent analysis to identify the fields new postdocs are pursuing. This may provide insight into areas of keen interest to early career researchers.
- ❑ Survey academic department heads or chairs responsible for hiring young faculty members. They have a good sense of what next generation scientists want to work on.
- ❑ Participate in multiple agency panels or discussions. A specific example is the series of Chemical Sciences Round Table discussions, including industry representatives, typically sponsored by the National Academies.
- ❑ Office of Science (SC) should continue to facilitate collaboration modes between and among DOE offices to leverage each other's research portfolio, avoid duplication, and challenge Principal Investigators to think outside the confines of their individual program office. It is important to think about how we should solve a scientific problem where multiple offices want the same outcome. PMs within the Office of Science could brainstorm how to convey that message with a unified voice. Methods for seamlessly progressing from fundamental work done by SC to more applied work e.g. Office of Energy Efficiency and Renewable Energy could be considered and if there are there gaps that need to be addressed jointly.
- ❑ Program Managers form small groups to pitch new areas to fund. They can defend the ideas to garner some initial funding for the new ideas.
- ❑ Track news and media for emerging areas of interest.
- ❑ Energy Frontier Research Centers could be areas to incubate new ideas. They could be given latitude and encouraged to use some of the research time outside of the original proposal concept.
- ❑ Create a Request for Information for emerging ideas. This could then motivate funding calls on those topics subsequently.

- ❑ At the national labs, the Laboratory Directed Research and Development (LDRD) programs may have valuable information about new ideas. For example, there is an annual reporting requirement for the funded programs, yet in addition to that information there may be other trends that emerge. For example, scanning topics of proposals that were not funded, sometimes due to lack of fit with existing programs, may provide insight into possible new areas of inquiry.

The report is available on-line at: www. science.osti.gov/bes/besac/Reports