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## External Evaluation of the Emergent Phenomena in Quantum Systems Initiative

## FINAL EVALUATION REPORT

Prepared for

The Gordon and Betty Moore Foundation Palo Alto, CA 94304

Prepared by

**RTI International** 3040 E. Cornwallis Road Research Triangle Park, NC 27709

Contact: Jeffrey Alexander, Ph.D. jalexander@rti.org +1 301.230.4656

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## **EXECUTIVE SUMMARY**

In 2017, RTI International was commissioned by the Gordon and Betty Moore Foundation (the foundation) to conduct an external, objective evaluation of its Emergent Phenomena in Quantum Systems (EPiQS) initiative. The first EPiQS grants were issued in 2013, and the program is budgeted to distribute \$90 million through 2019 to support research and related activities in the field of quantum materials. The purpose of RTI's evaluation is to:

- assess whether the strategies pursued by the EPiQS initiative were appropriate for achieving the desired outcomes and implemented effectively;
- identify the effects thus far of the EPiQS initiative's strategies on the quantum materials field of research; and
- generate observations on the initiative and its consequences, and how that might inform future investments in this field (or in comparable fields of research).

The EPiQS initiative is an integrated program of funding and activities intended to dramatically accelerate the pace of discovery in this field. The central motivation for EPiQS is encapsulated in its "Theory of Change," expressing how the initiative intends to make an impact on the field:

"By providing top scientists with access to the best materials and experimental probes, the resources and freedom to innovate, and opportunities to collaborate, EPiQS will catalyze transformative change in the science of emergent phenomena in quantum materials."

The key components launched as a part of EPiQS from 2013 to 2017 include:

- **Theory Centers:** Funding for universities recognized as leaders in quantum mechanics to hire postdoctoral scholars dedicated to the study of the theory of quantum materials.
- **Experimental Investigators:** Support for highly-accomplished Experimental Investigators to pursue ambitious and visionary research approaches to the characterization and measurement of these emergent phenomena.
- **Materials Synthesis Investigators:** Awards to researchers with proven expertise in the synthesis of samples of high-quality quantum materials, which can then be probed and studied by experimentalists.
- **Materials Synthesis Fellows:** Awards made to early-career (pre-tenure) faculty who showed dedication and potential to achieve advances in synthesis.
- **Equipment:** Grants supporting projects including the development of major new research user facilities serving the quantum materials community.
- **Rapid Response:** Grants to researchers who proposed particularly high-risk research plans that had potentially revolutionary impact on the field.
- **Community Building:** Grants for "community-building" programs supporting personnel exchanges and meetings for quantum materials researchers, plus sponsorship of other conferences and venues for scientific discussions.

The evaluation team broke down the topics covered into the six areas shown in **Figure ES-**. To do this, RTI engaged in three different streams of analysis:

- 1. Our *qualitative* analysis used structured interviews and document review to construct a retrospective narrative and analysis of how the EPiQS initiative developed and how its activities progressed over the past six years, and synthesized the opinions and recollections of grantees and other key stakeholders.
- Our quantitative analysis involved the deployment of a web-based survey to grantees and postdoctoral researchers supported by EPiQS. We gathered information about these individuals' activities and attitudes related to the initiative, providing trends and patterns in how EPiQS affected their research activities and accomplishments.
- Our scientometric analysis, conducted primarily by our research partner Observatoire des Sciènces et Technologies, used both state-of-the-art and exploratory methods of bibliometric and text analysis to make inferences about changes in research topics, publication behaviors, and community development in the quantum systems field.

#### Figure ES-1: Guiding Evaluation Topics

- 1. *Design* of the EPiQS Initiative (whether the strategies were appropriate to the objectives, and how the strategies might be improved)
- 2. *Implementation* of the EPiQS Initiative (whether the strategies were executed and managed properly, and any issues related to the conduct of the Initiative at the Foundation or among grantees)
- 3. *Researcher-level* impacts (effects of the Initiative on the behaviors and performance of grantees)
- Institution-level impacts (effects of the Initiative on the behaviors and activities of the institutions that employ grantees)
- 5. *Infrastructure-level* impacts (effects of the Initiative on the nature and availability of materials and equipment accessible to researchers)
- 6. *Community-level* impacts (effects of the Initiative on the overall community of researchers engaged in the study of quantum materials)

Separately, the foundation engaged an international *expert panel* of leading scientists in quantum materials, chaired by Dr.

Bernhard Keimer, Director of the Max Planck Institute for Solid State Research in Stuttgart, Germany. That panel evaluated the quality and impact of the scientific research undertaken by PIs and to identify potential future areas for scientific investment. The results of the expert review are also incorporated into this evaluation, especially as they relate to the six topics in **Figure ES-1**.

The RTI evaluation team conducted this evaluation study from approximately June 2017 through March 2018. As the EPiQS grants are mostly scheduled to end in 2019, the evaluation focused on summarizing progress to date and identifying early indicators of the initiative's impact.

## **PRIMARY EVALUATION FINDINGS**

After investigating the six evaluation topics, our analysis addressed three central issues most salient to the purpose of this evaluation:

- What progress has EPiQS made in realizing its short-term and long-term objectives?
- What has changed in the quantum materials research community since 2014, and what aspects of that change might be attributable to the funding and activities of EPiQs?
- In light of those changes, what options might be considered in decisions about future support for quantum materials research?

#### Measuring the Progress of EPiQS Against Its Theory of Change

Using the Theory of Change above as the framework for assessing the implementation and immediate impacts of EPiQS, we found the following:

- "...providing top scientists... " -- Stakeholder interviews, the expert panelists, and analysis of publications all indicate that the EPiQS grantees are representative of the most accomplished and prominent researchers in empirical experimentation and materials synthesis. While it's arguable that there are nongrantees equally accomplished to the Investigator grantees, no one has stated that the cohort of grantees had anyone undeserving of support.
- "...access to the best materials and experimental probes... " Our analysis shows that EPiQS funding supports important work by key specialists in materials synthesis, both in the production of new materials and in optimizing the quality of materials in high demand (for example, the work by Loren Pfeiffer to improve the quality of gallium arsenide). Also, while the Equipment Development grants are bound to create important new major facilities for measurement and characterization, all investigators invested in new equipment and instruments for their own laboratories. Such purchases are much more difficult to make using federal funding. That equipment benefits the grantees research supported by EPiQS, but also will benefit research supported by other sponsors, and give postdoctoral researchers and graduate students training on the latest technologies in materials characterization and synthesis.
- "...the resources and freedom to innovate..." Grantees were afforded substantial latitude in how they chose to carry out their research, and in changing their research direction to pursue new discoveries and interests. Combined with the scale and duration of the awards, the investigators were able to take on research goals very different from what is possible using more conventional federal funds.
- "...opportunities to collaborate..." -- As indicators of progress on this point, EPiQS awardees reported that they formed new research partnerships with other awardees, and also with nonawardee scientists (such as visiting scholars sponsored by EPiQS), and that they felt it unlikely that they would have made those contacts or identified those collaborative projects without EPiQS. The new collaborations can be seen in the large number of joint publications coauthored by EPiQS grantees, and changes in the nature of their research collaborators when compared to their work before EPiQS. Not only were grantees presented with a range of opportunities to collaborate; they took advantage of those opportunities, leading to productive and valuable results.

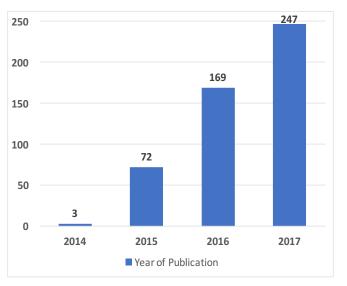
Our findings indicate that the design of the EPiQS initiative was well-suited to enable advances in the science of quantum materials, and that it targeted very specifically perceived deficiencies in the U.S. research environment that seemed to prevent the most accomplished scientists from realizing the full potential of their research.

#### Assessing the Role of EPiQS in Transforming the Field of Quantum Materials

The ultimate goal of EPiQS is to "catalyze transformative change" in the science of quantum materials. A challenge for the initiative is that the term "transformative change" is not easily defined. If the envisioned "transformative change" is a set of fundamental discoveries that revolutionize the understanding of this domain, it is important to recognize that such fundamental discoveries often take years to appear. In addition, their actual transformative impact may not be realized and evident for an even longer period.

Due to the period required to launch new investigations with their awarded funds and the typical publication review cycles, articles reporting the results of EPiQS-funded research are just now appearing en masse in the scientific literature, shown in **Figure ES-2** (using data from the Web of Science database provided by Clarivate Analytics). In light of this, the four years since the first EPiQS awards is too short a period to identify truly "transformative" discoveries or advances that might be attributable to EPiQS funding. The expert panel did





identify multiple instances where early research results from EPiQS awardees generated excitement and interest in the community. The panel also noted new techniques and instruments under development by grantees that when completed and tested could provide revolutionary capabilities in materials synthesis and characterization. We can say that EPiQS may have catalyzed scientific results that are potentially transformative, but without certainty about whether and when they would realize that potential.

The evaluation documented key changes in the U.S. research environment that can be reasonably thought to enable creative and innovative research efforts, and to encourage grantees to pursue and realize radical advances in discovery and understanding. Based on our analysis of the data collected for this project, we argue that the following changes in the U.S. quantum materials research community were substantially influenced by EPiQS:

#### EPiQS aided in establishing "quantum materials" as a distinct field of science.

Stakeholders in the condensed matter and materials physics community report that they have a more coherent view of what "quantum materials" means, as a field of research. While EPiQS did not coin that term, our research indicates that EPiQS raised its profile, and helped to bring together the community of researchers studying that field. The recognition of this field, encouraged by EPiQS, makes it easier to identify scientific advances relevant to this field, track the members of the community and their research products, and allocate funding specifically to quantum materials research.

EPiQS grew the pipeline of researchers entering the field of quantum materials

**research.** Doctoral students and postdoctoral researchers are directing their research interest towards quantum materials, fueling the future research community in this field. The EPiQS initiative's support for the theory postdocs, and the support for postdocs working with EPiQS Investigators, expanded opportunities for talented young researchers to enter this field and launch their careers. Almost all former postdocs working in theory or in experimentation and synthesis have gained permanent employment as university faculty or scientists in prominent research institutes, with about half of them landing at U.S. institutions.

**EPiQS raised the standing and significance of materials synthesis as a key part of the U.S. research community.** Research in quantum materials is enabled by the capacity to synthesize high-quality samples of such materials for experimentation and study. For various historical reasons, U.S. capabilities in synthesis eroded over the past two decades, and researchers specializing in synthesis faced serious challenges in gaining faculty positions in physics. EPiQS brought new attention to this important aspect of physics by providing substantial and highly visible support to leading U.S. researchers in synthesis, and subsequently expanding the capacity for those researchers to provide sample materials to empirical investigators. Today, there is evidence of growing interest at universities and federal research agencies to invest in new synthesis labs and researchers, and there is broader recognition of the importance of this particular research specialization.

**EPiQS contributed to decisions to hire new faculty in materials synthesis.** Based on views expressed by leaders and members of the physics faculty of major U.S. universities, the EPiQS awards to synthesists facilitated efforts to expand academic positions for such researchers. Hiring a faculty member in materials synthesis requires a significant upfront cost for a university, as they need specialized research environments and expensive equipment. The funding provided to the Moore Fellows in Materials Synthesis, early-career researchers focused on synthesis, mitigated that barrier, facilitating the process of hiring those Fellows into tenure-track positions.

Other research sponsors are interested in supporting quantum materials research, especially in tandem with EPiQS. Historically, most of the funding for research in areas

like quantum materials has been provided by federal science agencies, especially in the Department of Energy (DOE), Department of Defense (DOD), and National Science Foundation (NSF). Almost all EPiQS awardees report that the research supported by their awards helped them to win additional research funding from outside sponsors, and we have documented examples of EPiQS investigators gaining new funding awards directly tied to the topics of their EPiQS proposals. The DOE and NSF believe that by supporting EPiQS investigators, they are able to leverage their own resources and further enable those researchers to pursue fundamental new knowledge. The EPiQS initiative has succeeded at least partially in achieving synergistic effects with other funding sources.

### CONSIDERATIONS FOR THE FUTURE OF SUPPORT IN QUANTUM MATERIALS RESEARCH

Our findings establish that the environment for research in quantum materials has improved, at least for leading researchers targeted by EPiQS. EPiQS played a role in those changes, although the full impacts of the initiative are still unfolding. The research conditions in quantum materials in 2019 are different from how they stood in 2012, when EPiQS was conceived. Therefore, the foundation may want to consider additional mechanisms for supporting quantum materials research, if it chooses to extend such support.

**Ending EPiQS without a follow-on program would undermine its impact.** Our evaluation identified clear signs that EPiQS improved research conditions in the U.S. quantum materials community in ways that are likely to endure beyond the current funding period. These improvements do not necessarily constitute "transformative change," however, and there is little evidence that the changes are sustainable without some ongoing support. Furthermore, EPiQS generated substantial interest in the field of quantum materials due to the reputation and resources of the Gordon and Betty Moore Foundation. Almost all stakeholders interviewed, including nongrantees and federal research program managers, feel that discontinuing the efforts launched under EPiQS would be viewed as a "vote of no confidence" in the value of quantum materials research. Younger researchers and research funders could reduce their interest in this field as a result. Terminating the EPiQS program in 2019 with no formal follow-on program could negate its contribution to the field.

**Growing the EPiQS community is feasible, but with caveats.** EPiQS clearly succeeded in its aim to select as grantees a group of highly-accomplished researchers with substantial potential. Researchers in the field, including grantees, agree that EPiQS could have increased the number of grantees by perhaps 50% without sacrificing the overall quality of the grantee pool. Expanding the number of grantees in the future could increase opportunities for collaboration, add more support and mentorship for postdocs and other

young researchers, and bring more capable researchers with potentially transformative ideas into the initiative. Those benefits are countered by at least two issues. First, the current funding amount per award is calibrated to the type of research that EPiQS aims to support. Increasing the number of awards by decreasing the average funding level would be counterproductive. Also, expanding the number of grantees might change the dynamics if the annual Investigator Symposium, considered by grantees to be a major benefit of the initiative. Hosting more participants at the Symposium would make it more difficult for program staff to manage discussions, and would also give each grantee fewer opportunities to have in-depth conversations with a significant number of other grantees. This argues for at most a moderate increase in the number of researchers supported.

Supporting a broader range of researchers may be beneficial, but would increase program-level risk. EPiQS awards were granted predominantly to researchers at U.S. universities with the greatest funding for physics R&D. This is consistent with the Theory of Change, as institutions with such resources are most likely to attract the top researchers in quantum materials. At the same time, this may limit the initiative, as it may fail to identify and support promising researchers who happen to be at less-prestigious institutions. Even a more modest award to such researchers would provide them with substantial benefits to pursue their boldest ideas. Some stakeholders interviewed felt that EPiQS could benefit from including such "hidden gems" into the pool of grantees. Since many EPiQS grantees knew one another before their awards, funding less-prolific but capable researchers could inject "new blood" into the grantee pool. Still, attempts to support such researchers must address two issues. EPiQS would need to develop new approaches that would identify such researchers, as their more modest stature makes it difficult to submit them to the same review process used in previous awards. EPiQS would also increase its overall risk as researchers with fewer recognized achievements and lower resources may not have sufficient experience to manage the uncertainty integral to highly-risky research approaches. Supporting a small number of such researchers could be pursued opportunistically, affording those researchers adequate access to program staff and their more experienced colleagues for advice and guidance.

**Individual investigator awards are still preferable to funding multi-PI research centers.** Given that EPiQS aims to encourage collaboration among researchers in quantum materials (including collaborations involving nongrantees), some stakeholders were surprised that no funding was devoted to research centers that could organize larger teams of PIs in more formal joint research initiatives. Even at institutions housing multiple grantees, EPiQS funds are distributed as single-PI awards. The dominant view of stakeholders is that with a single-PI approach, EPiQS promotes collaborations formed entirely at the discretion of each grantee, based on that grantee's interests and needs. This approach provides more flexibility and less administrative burden compared to funding awarded to a formal collaborative research organization.

#### Funding experienced PIs through EPiQS benefits new researchers entering the

field. With the exception of the Theory Center awards and the Moore Fellows in Materials Synthesis, all EPiQS funding provided direct support to faculty who were for the most part well-established in the field. Even so, perhaps the most consequential investments enabled by EPiQS are the postdocs hired by grantees with EPiQS funds. Many stakeholders lauded the record of EPiQS in growing the pipeline of talent into quantum materials. Tracking the future careers of postdocs in particular could capture an important dimension of the initiative's impact. A few stakeholders cautioned that EPiQS may be "distorting" the pipeline by supporting so many postdocs in that they exceed the number of openings for tenuretrack faculty and permanent researchers in this field. We did not find any evidence that EPiQS funding would lead to a "glut" in the postdoc population (a condition that has occurred in the biomedical research community). To date, postdocs hired at Theory Center institutions or by investigators enjoy very promising job prospects when they transition out of those postdoctoral positions. Almost all end up as tenure-track faculty at research universities, or permanent research staff at prestigious stand-alone research institutes. These postdocs are better prepared to become the next generation of leading quantum materials researchers thanks to their association with the EPiOS initiative.

**EPiQS has not changed the behaviors of other research sponsors—yet.** One aspiration of EPiQS is that by focusing more attention on quantum materials research, other major sponsors will recognize the value of this field and boost their own investments in similar research. The NSF and DOE, two of the most prolific sponsors of research in condensed matter and material physics, have issued reports and announcements showing that quantum materials research is now a priority in their programs. However, given the current federal fiscal environment, there is only limited new money to invest in such research. In contrast to EPiQS, federal funding agencies distribute more funding per year, but to a much larger number of awardees with smaller funding amounts of more limited duration. Not only are the agencies unable to add funding to match the investment in EPiQS, their programs have more rigid administrative procedures and guidelines that make them less conducive to supporting high-risk, potentially transformative research.

Still, given time and resources, federal agencies are capable of innovation in their funding mechanisms. Despite their history of funding research on a project-by-project basis, some federal agencies are experimenting with programs that provide consistent and stable funding to selected top researchers. Examples of such agencies include the National Institutes of Health and the Army Research Office. The current time horizon on EPiQS is too short to observe such change in federal agencies. In another five to fifteen years, the community of funders of quantum research may grow and evolve so that their research portfolios be used to catalyze the type of transformative research targeted by EPiQS.

## 1. INTRODUCTION: THE EPIQS INITIATIVE EVALUATION PROJECT

In July 2013, the Gordon and Betty Moore Foundation issued its first grant under its Emergent Phenomena in Quantum Systems (EPiQS) initiative. 49 principal investigators (PIs), based at 21 institutions in the U.S. and three in Canada, have received awards ranging from approximately \$300,000 to over \$4 million each in an integrated effort to achieve two key goals: improve research conditions in the U.S. for investigators focused on quantum materials, and enable its investigators to generate fundamental scientific advances and discoveries that could transform the entire field. By the end of its current timeline, EPiQS will have distributed over \$84 million in direct research funding across 51 awards.

In 2017, the Gordon and Betty Moore Foundation commissioned RTI International to conduct an external, independent evaluation of EPiQS. The RTI evaluation team conducted this study between June 2017 through March 2018. Most EPiQS grants are scheduled to end in 2019. As such, the evaluation focused on assessing progress to date and identifying early indicators of impact on the quantum materials research community attributable to this initiative.

The foundation launched EPiQS due to the potential significant impact that could be gained from advancing knowledge about the nature of quantum materials. Although there is no canonical definition of the term *quantum materials* as yet, this label encompasses the study of how particular materials under the right conditions manifest unique properties and behaviors that cannot be explained through classical subatomic physics. The particular characteristics of this field make it especially ripe for potentially-transformative advances, and also provide conditions where the foundation's targeted investments and activities could spur dramatic change in the U.S. research community in particular. In turn, it may influence the global community of quantum materials researchers.

The purpose of the evaluation was to:

- assess whether the strategies pursued by the EPiQS Initiative were appropriate for achieving the desired outcomes;
- determine if the EPiQS Initiative implemented its strategies effectively;
- identify the *effects* thus far of the EPiQS Initiative's strategies on the quantum materials field of research; and
- generate observations on the current state of the U.S. environment for quantum materials research, and how that might inform future investments in this field.

# **1.1** Context: Quantum Materials Research in the U.S. in the Early 21<sup>st</sup> Century

To understand the significance of quantum materials, and the potential impact of the EPiQS Initiative on this field, we review first some of the key characteristics of the science of quantum materials and describe briefly the conditions in the U.S. research environment addressed by EPiQS.

Quantum materials are a broad group of materials that exhibit patterns of subatomic behavior that are only explicable through our understanding of quantum mechanics (see box, Quantum Materials **Defined**). The properties that result from these behaviors could, if understood and harnessed properly, become the basis for revolutionary technologies with substantial economic and other benefits. For example, superconductivity has been observed in a range of materials, but only at very low temperatures by human standards (less than 140 kelvin), or -130°C. If scientists could discover or develop a superconductor operating at close to room temperature, this would open the possibility of developing superconducting power lines that could transmit electricity with zero loss, dramatically increasing the capacity of the national power grid.

#### **Quantum Materials Defined**

Quantum materials are solid materials and artificial structures in which complex interactions among constituent electrons lead to a variety of emergent phenomenacooperative behaviors that cannot be predicted from the properties of individual electrons. Many of these phenomena-such as hightemperature superconductivity (flow of electricity with zero resistance), and the appearance of "emergent particles" that do not resemble any real particle—are only beginning to be understood. These phenomena can be understood through laws of quantum mechanics but cannot be explained by the laws of classical physics.

At the start of the 21<sup>st</sup> Century, the field of quantum materials presented new opportunities for discovery resulting from simultaneous advances in three aspects of this science:

- Theorists in quantum mechanics, who (as one interviewee stated) primarily "work in their heads," developed new theoretical frameworks and models that showed promise in explaining the emergence of unusual quantum phenomena. Tools for computational simulation are growing in utility and importance in this area.
- New varieties of instrumentation, with the ability to detect features and dynamics at increasingly minute scales, now provide empirical researchers with the ability to make new observations about quantum behaviors and properties in materials. This drives the discovery of new types of phenomena, and the data to inform theorists on potential explanations.
- Capabilities in materials synthesis, supported by new types of equipment to manipulate elements in precise fashion, now produce more exotic and interesting samples of materials. Recent innovations range from graphene, a material derived from graphite that exists primarily in two dimensions, to crystals that combine elements in ways not found in nature.

As noted in a 2014 report by a subcommittee of the Advisory Committee to the National Science Foundation's Directorate for Mathematical and Physical Sciences, these opportunities could be realized much more rapidly by "tightly closing the loop among synthesis, characterization, theory/modeling and targeted materials outcomes."<sup>1</sup>

At the same time, observers in this field noted troubling signs in the U.S. research environment for quantum materials. A "decadal survey" of condensed matter and materials physics in the United States, conducted by a panel of the National Academy of Sciences in 2006 and 2007, summarized the challenges that threatened to degrade this environment.<sup>2</sup>

- University-based researchers who pursued this field found that federal government grant awards were becoming less effective, as the typical award size did not increase at a rate commensurate with rising research costs.
- Federal research programs seemed to grow more rigid, as concerns about demonstrating "performance" led some program managers to impose shorter-term metrics on investigators (e.g., the volume of articles published per year).
- The withdrawal of the large industrial labs (primarily IBM's research facilities and AT&T's Bell Laboratories) from the field in the 1990s greatly restricted a key research input—access to high-quality samples of the synthesized materials that researchers could study to investigate and understand the nature of quantum materials.

The Gordon and Betty Moore Foundation conceived and launched EPiQS in this atmosphere of scientific opportunity and systemic challenges. During interviews for this study, researchers and other key stakeholders in the field asserted consistently that U.S. academic researchers, even at the most prestigious and advanced universities, were at a disadvantage to their peers in Europe and Asia as dominant (federal) funding mechanisms were not evolving to counteract those challenges. In addition, U.S. researchers in quantum materials seemed to lack a cohesive sense of community, as they were separated by both the geographic distance between leading research institutions and long-standing boundaries between subdisciplines, areas of expertise, and academic departments.

## **1.2** Rationale and Structure of the EPiQS Initiative

The EPiQS Initiative provides resources and activities designed to stimulate ground-breaking advances in quantum materials research, in part by reducing the systemic barriers that

<sup>&</sup>lt;sup>1</sup> See MPSAC Subcommittee on Materials Instrumentation. (2014). *Closing the loop*. Arlington, VA: Directorate for Mathematical and Physical Sciences, National Science Foundation.

<sup>&</sup>lt;sup>2</sup> National Research Council (U.S.) Board on Physics & Astronomy (2010). *Condensed-Matter and Material Physics: The Science of the World Around Us.* Washington, DC: National Academies Press.

seem to hamper such research. The program rationale is expressed in a "Theory of Change" developed at the launch of the program in 2013:

*By providing top scientists with access to the best materials and experimental probes, the resources and freedom to innovate, and opportunities to collaborate, EPiQS will catalyze transformative change in the science of emergent phenomena in quantum materials.*<sup>3</sup>

The Theory of Change captures the key postulates underpinning the strategies employed by EPiOS:

- History shows that it is extremely difficult to predict which scientists will make specific ground-breaking discoveries in a given field of science. In practice, such breakthroughs in science tend to be produced by a small number of the most talented and creative people in that field. This is particularly true in quantum materials, where experienced researchers have both the perspective and expertise to identify promising research pathways and determine how to pursue them.
- The availability of high-quality materials and leading-edge experimental probes are necessary conditions for rapid progress in this field. This means that the best empirical work requires access to advanced instrumentation and concurrent access to a reliable and relatively close source of sample materials. Shipping samples of quantum materials over long distances can increase the chances of mishandling or other factors that cause defects in the material, undermining the validity of experiments conducted with those materials.
- Top scientists can achieve maximum creativity and output when provided with (a) adequate and sustained funding; (b) flexibility to change research directions when warranted by surprising results, developments in the field, or their intuition; and (c) a collaborative environment within a community of scientists of similar caliber.<sup>4</sup> The recent history of science indicates that high-performing research organizations provide that type of environment and attract the best researchers. The most prominent example of this in condensed matter and material physics was the environment at AT&T Bell Labs from the 1940s through the 1980s, which produced some of the most consequential discoveries in materials (such as the transistor).<sup>5</sup>

The bulk of EPiQS funding was invested in research grants in three areas: theory, experimentation, and materials synthesis.

 Six universities received *Theory Center* awards. These universities were selected from 12 institutions judged to have the most prominent programs in quantum mechanics theory applied to the study of materials. The awards enabled each university to support two to four new postdoctoral researchers per year, the Moore Postdoctoral Scholars in the Theory of Quantum Materials. Those scholars then worked with the theory faculty at those universities, and other collaborators around the world, to establish conceptual frameworks to inform experimentation and

<sup>&</sup>lt;sup>3</sup> Gordon and Betty Moore Foundation. (2015). *Final EPiQS strategy review Appendix I - Updated Initiative revised 2015*. Palo Alto, CA: Gordon and Betty Moore Foundation, p. 4. <sup>4</sup> Ibid.

<sup>&</sup>lt;sup>5</sup> For background, see Gertner, J. (2015). *The Idea Factory: Bell Labs and the Great Age of American Innovation.* Penguin Press: New York, NY.

improve the interpretation of results. The centers also host visiting scholars focused on the theoretical aspects of quantum materials.

- 19 researchers were selected as *Experimental Investigators*, after a rigorous competition in response to an open call for proposals. These PIs received awards based primarily on two criteria. First, each of their proposals described an innovative and ambitious research vision that, if fulfilled successfully, was likely to spur broad-based and rapid progress in understanding quantum materials. Second, each PI had demonstrated scientific achievement over the past 8 to 10 years such that the EPiQS initiative could have confidence that they were capable of achieving such ambitious goals or redirecting their research to the most promising opportunities for discovery.
- EPiQS awarded 12 Synthesis Investigator grants from a select pool of invited proposers encompassing recognized leaders in the production and sharing of samples of high-grade quantum materials. For reasons discussed later in this report, research in materials synthesis is an area thought to require emphasis and support in the U.S. In addition to these 12 PIs, who are primarily mid-career or senior faculty members at their institutions, EPiQS named four *Moore Fellows in Materials Synthesis*. These were junior tenure-track faculty who showed promise in pioneering new methods in synthesis.<sup>6</sup>

EPiQS also made separate awards for projects expected to offer important contributions to the field of quantum materials research.

- Five *Equipment Development Grants* (often with cost-sharing contributed by recipient institutions) support the design and installation of major new facilities and equipment offering revolutionary improvements in the ability to characterize and measure quantum materials.
- Five *Rapid Response Grants* were given to PIs in response to compelling and timely proposals submitted outside of the Experimental Investigator and Synthesis Investigator grant competitions. These PIs proposed particularly high-risk research projects that are aimed at achieving uniquely impactful results.
- Finally, four *Community-Building* grants were awarded to PIs at organizations that facilitate scientific exchanges, information-sharing, and collaboration by hosting visiting scientists and workshops and meetings targeting the quantum materials research community. Examples of such organizations include the Canadian Institute for Advanced Research (CIFAR) based in Toronto, and the Institute for Complex Adaptive Matter at the University of California at Davis.

Other notable investments by EPiQS were made to promote a more cohesive global community of quantum materials researchers include:

 An annual Investigator Symposium, where PIs gather for 3 to 5 days of intensive presentations and discussions. The three symposia held to date (in 2015, 2016, and 2017) took place in California at the end of July or early August. Investigator awardees are required to attend the symposium, and most other EPiQS PIs also join in that meeting, as well as selected guests.

<sup>&</sup>lt;sup>6</sup> The EPiQS Initiative announced the selection of two additional Moore Fellows in Materials Synthesis October 2017 and February 2018, after the start of the evaluation. These awardees are not included in this evaluation report.

- A Postdoctoral Symposium, where postdoctoral researchers supported through the Theory Center and other awards (along with some graduate students) can present their work to one another without any faculty participants.
- Co-sponsorship of more widely-attended conferences, workshops, and summer and winter schools exploring topics in quantum materials research, as well as specialized media promoting the ideas and significance of quantum materials.

Taken together, these components of the EPiQS initiative offer multiple mechanisms that can enable transformative change in the way that quantum materials research is conducted, as well as in the understanding of quantum materials. However, the time scale and mechanisms of transformative change in science are not amenable to a straightforward evaluation. New discoveries occur at irregular and unpredictable intervals, and often the full significance of a discovery is not realized until years or decades after it occurs. Scientific research is also an activity where failures to achieve experimental results can be valuable as learning experiences that contribute to the knowledgebase of the field. These factors affected the design of RTI's evaluation approach, which is summarized in the following section.<sup>7</sup>

## **1.3 Evaluation Approach and Methods**

The EPiQS initiative is still an active program, and the full course of the program have yet to be completed. Therefore, this evaluation cannot produce a definitive summary of its total impact, as that may take years to be realized. Instead, this evaluation captured historical and contemporaneous data on activities, people, and events related to the EPiQS initiative in an effort to discern early and emerging signals of its likely effects. We used three primary modes of data collection and analysis:

- 1. The *qualitative* analysis employed structured interviews and document review to construct a retrospective narrative and analysis of how the EPiQS initiative developed and how its activities progressed since approximately 2012. Based on interview transcripts and notes, supplemented by primary documentation, we synthesized the opinions and recollections of grantees and other key stakeholders to provide a detailed, qualitative assessment of the initiative. For this report, over 100 individuals were interviewed, spanning categories that include grantees, non-grantee funding applicants, journal editors in quantum materials, department chairs of EPiQS-funded institutions, graduate student and postdoctoral researchers supported by EPiQS grants, and federal research program managers.
- 2. The *quantitative* analysis involved developing and deploying two web-based surveys: one for grantees and one for funded postdoctoral researchers. We used the surveys

<sup>&</sup>lt;sup>7</sup> For further discussion of these dynamics, see works such as Cozzens, S. E. (1997). The knowledge pool: Measurement challenges in evaluating fundamental research programs. *Evaluation and Program Planning*, *20*(1), 77—89; and Ke, Q, Ferrara, E., Radicchi, F., & Flammini, A. (2015). Defining and identifying Sleeping Beauties in science. *Proceedings of the National Academy of Sciences of the United States of America*, *112*(24), pp. 7426–7431.

to gather short structured and open-ended responses to a standardized set of questions about the initiative and those respondents' activities and characteristics. We then used statistical analysis to detect broader patterns of behavior across those individuals and their institutions. Of the 59 grantees surveyed, 46 returned responses sufficiently complete for our analysis. For postdocs, 47 researchers were surveyed, of whom 36 provided sufficiently complete responses.

3. A *scientometric* analysis was conducted by our research partner, the Observatoire des Sciènces et Technologies at the University of Quebec at Montreal. This used both state-of-the-art and exploratory methods of bibliometric and computational text analysis to make inferences about changes in research topics, publication behaviors, and community development among EPiQS grantees and in the broader quantum systems field.

The evaluation team also interacted with an international panel of subject matter experts in quantum materials convened by the foundation (see box, Members of the Expert Panel). As recognized leaders engaged in quantum materials research themselves, the panel members were able to assess the quality of the research undertaken by grantees and the present and potential scientific impact of their investigations and discoveries. The panel also commented to some degree on operational aspects of the initiative. This report integrates some elements of the expert panel findings, especially in how the design and implementation of EPiQS may have contributed to the scientific achievements of grantees.

#### Members of the Expert Panel

Bernhard Keimer, Director, Max Planck Institute for Solid State Research, Stuttgart, Germany

Andrea Cavalleri, Director, Condensed Matter Department, Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany and Professor of Physics, University of Oxford, United Kingdom

**Yoshiteru Maeno**, Professor, Department of Physics, Kyoto University, Japan

**Alberto Morpurgo**, Professor, Department of Quantum Matter Physics, University of Geneva, Switzerland

**Gil Refael**, Taylor W. Lawrence Professor of Theoretical Physics, California Institute of Technology, Pasadena, CA

**George Sawatzky**, Professor of Physics & Chemistry, University of British Columbia, Vancouver, BC, Canada

Specific details of the methodologies, data

sources, and findings for each of these three analyses can be found in their respective analytical reports, incorporated here by reference.

In planning this evaluation, we presented a list of 24 guiding evaluation questions to be addressed by this project, grouped under six themes (see **Figure 1-1**):

- design of the EPiQS Initiative
- implementation of the EPiQS Initiative
- researcher-level impacts
- institution-level impacts
- infrastructural impacts
- impacts on the quantum research community

#### Figure 1-1. Detailed Guiding Evaluation Research Questions

#### 1. EPiQS Design

- 1.1. How did the design of the EPiQS Initiative differ from existing sources of support for quantum materials research?
- 1.2. Did the original design of the EPiQS Initiative address recognized needs of the quantum materials research community?
- 1.3. Did the strategies offer appropriate modes of support for the desired outcomes?
- 1.4. What were the implications of **not** using a different set of funding approaches?
- 1.5. Do the initiative's intended outcomes provide an actionable framework for measuring progress and for determining the success of the program when it ends?

#### 2. EPiQS Implementation

- 2.1. Was the EPiQS Initiative implemented in a manner consistent with its design?
- 2.2. If implementation differed from the original design, were those changes made for justifiable reasons?
- 2.3. What has the EPiQS program staff learned in the process of implementing the initiative?
- 2.4. Has the implementation provided the proper degree of oversight and freedom to grantees?

#### 3. EPiQS Impact: Researcher Level

- 3.1. How has EPiQS support changed the focus and conduct of research by grantees?
- 3.2. In what ways do grantees feel that EPiQS support has advantages or disadvantages relative to other forms of funding?
- 3.3. To what extent are EPiQS-supported researchers changing their patterns of research collaboration?
- 3.4. How has EPiQS funding affected the career trajectories of the Moore Fellows in Materials Synthesis and the Moore Postdoctoral Scholars in the Theory of Quantum Materials?

#### 4. EPiQS Impact: Institutional Level

- 4.1. Are the institutions that received EPiQS support more inclined to train or hire researchers specializing in materials synthesis?
- 4.2. To what extent has EPiQS support enhanced the capacity of funded institutions to conduct research in quantum materials, particularly for those housing multiple grantees?
- 4.3. Has the support for the Moore Postdoctoral Scholars at Theory Centers changed the way that research is carried out at those institutions?

#### 5. EPiQS Impact: Infrastructure Level

- 5.1. To what extent is EPiQS support expanding the locations and capacity for materials synthesis in the U.S.?
- 5.2. How is the acquisition or development of equipment through EPiQS support expected to benefit future research in this field?

#### 6. EPiQS Impact: Community Level

- 6.1. How does the research pursued by EPiQS grantees compare to other research in this field?
- 6.2. To what extent are EPiQS-supported researchers introducing new research topics, concepts, theories, and tools to the community?
- 6.3. Is EPiQS support changing the patterns and prevalence of collaboration across institutions and in the broader quantum materials community?
- 6.4. Has EPiQS had an effect on the support and programs of other sponsors that traditionally fund research on similar topics?
- 6.5. Has EPiQS helped to establish "quantum materials" as a distinct field of research?

# 2. DESIGN OF THE EPIQS INITIATIVE: AN INNOVATION IN THE SUPPORT OF PHYSICAL SCIENCES RESEARCH

In this section, we review the factors contributing to the decision to launch the EPiQS Initiative and how those shaped the design of the initiative. These factors influence why and how EPiQS had the effects documented in later sections of this report.

#### Key Findings

- The EPiQS funding strategies used innovative approaches, such as basing awards on particular investigators rather than discrete projects, to address opportunities and needs facing the U.S. quantum materials research community.
- The EPiQS initiative's scale and scope were sufficient to achieve the desired impact.
- The metrics and ultimate objectives of EPiQS could be aligned more closely with the Theory of Change.

## 2.1 Aligning EPiQS with Conditions in the U.S. Quantum Materials Research Environment

As noted in the Introduction, the field of quantum materials research faced opportunities and challenges in the early 2000s. The opportunity in quantum materials was driven by advances in theory, empirical experimentation, and materials synthesis. At the same time, the research funding environment in the U.S. posed challenges to researchers in those areas:

- Theorists in quantum materials use their individual and collective insights to devise conceptual frameworks and theories explaining the quantum dynamics of emergent phenomena. Graduate students and especially postdoctoral researchers are vital assets to theorists. The size of research awards in this area, especially from the NSF, has barely kept pace with inflation, while the cost of supporting students and postdocs has risen considerably faster than inflation. At major universities, NSF awards can cover only partially the cost of a student, and rarely the cost of a postdoc. At the same time, new innovations in computational tools require theorists to relearn how to formulate new theory based on empirical results.
- Empirical experimentation in quantum materials, in contrast, relies heavily on sophisticated instruments and equipment to handle materials properly and collect measurements. In addition to tight funding conditions, researchers who accept federal funds face substantial administrative requirements and rigid performance goals imposed in the name of accountability. This requires researchers to focus on projects that emphasize incremental advances and short-term results, when the greatest opportunities require sustained effort and dynamic approaches.

 Materials synthesis is not well supported in U.S. academic physics departments. For faculty outside this domain, synthesis might appear more like engineering rather than research. Also, synthesis requires expensive infrastructure and intensive training that is not strictly scientific. One synthesist described his work as a combination of science and fine cooking, where elements are mixed and manipulated in part by detailed knowledge of their characteristics and in part by gut instinct. Researchers specializing in synthesis routinely faced roadblocks in finding institutions willing to hire them and provide them with the necessary laboratory environment to produce high-quality materials.

Based on information from individuals involved in the early planning of EPiQS, the initiative's awards were structured by the program staff to avoid the challenges inherent in federal funding programs. For theorists, the Theory Center awards enabled those institutions to hire postdoctoral scholars focused on quantum materials theory, but without the need to conform to a particular PI's research interest. The Experimental Investigator awards provided substantial funding over an extended period (\$1.8 million over 5 years) to plan and execute a more ambitious research agenda. In synthesis, the Synthesis Investigators likewise enjoyed substantial funding (\$1.5 million to \$1.9 million) over a five-year term, while the Moore Fellows in Materials Synthesis could use their awards (\$1.2 million to \$1.5 million) to supplement any start-up funding they received from their new institutions. In a different sense, the more variable Rapid Response grants (\$650,000 to \$1.5 million) provided timely support to researchers with innovative and unconventional research approaches that might otherwise be rejected by federal funding agencies.

The consensus view of stakeholders interviewed for this evaluation, along with comments from the expert panel, is that for EPiQS grantees, the funding that they receive puts them closer to parity with the favorable research conditions enjoyed by world-class researchers in Western Europe and the advanced Asian nations.

## 2.2 Calibrating the EPiQS Investment to the Intended Impact

U.S. federal science agencies spend a considerable amount of funds to support research in condensed matter physics and other disciplines related to quantum materials research. Unfortunately, it is not possible to make an accurate estimate of federal spending on the science of quantum materials, because "quantum materials" is not a recognized category of spending in federal budget terminology. To produce a reasonable estimate, we combined figures provided by program managers during interviews with public grant records downloaded from the DOE and NSF web sites for the years 2015 to 2017. By this estimate:

 DOE, which supports research in areas like quantum materials through its Office of Basic Energy Sciences, issues 30 to 40 awards per year for total spending of \$15 to \$20 million annually. Note that this figure *excludes* funding for similar work conducted by researchers at the DOE National Laboratories. That work is accounted for in a different manner and not readily accessible. Typical awards amount to \$400,000 to \$700,000 over 3 to 4 years.

 The NSF invests in quantum materials research through programs in its Division of Materials Research, along with the Chemistry and Physics Divisions. Those programs issue between 100 and 140 awards per year, totaling \$25 to \$30 million per year. Note that this excludes funding for the Materials Research Science and Engineering Centers, some of which conduct quantum materials research, and that it includes funding for workshops, conferences, summer institutes, and similar meetings. Typical awards are \$200,000 to \$300,000 over two years.

The third source of basic research funding for the physics of materials is the Department of Defense. The specific funding sources are the service arm science agencies: chiefly the Army Research Office, and to a lesser extent the Air Force Office of Scientific Research and the Office of Naval Research. Extramural funding amounts from these sources is too difficult to obtain, but anecdotal input estimates that each office spends no more than \$5 million annually on research relevant to quantum materials. In addition, they issue awards to a smaller number of investigators and over longer timeframes compared to the civilian funding agencies.

Taken together, these five agencies invest roughly \$50 million to \$100 million each year to support external researchers in fields related to quantum materials. In contrast, the budget of EPiQS (\$90 million total spread across five years) seems relatively small. However, that comparison involves some important caveats:

- EPiQS supports a much smaller number of investigators with much larger awards over longer timeframe. The federal agencies are funding hundreds of PIs (as awards go to different sets of PIs each year), compared to less than 50 for EPiQS. The value of EPiQS to its funded researchers is much greater.
- Most institutions charge an indirect cost fee when accepting research awards. At major research universities, the indirect rate is generally at least 50% (meaning that \$0.66 of each award dollar goes to actual research activities) and can range as high as 80%. The Moore Foundation only allows institutions to charge an indirect rate of 12.5%. This means that a much greater ratio of each EPiQS award is spent directly on research. (Universities argue that they are subsidizing in effect each EPiQS award.)
- As discussed in the next section, PIs have substantial discretion over how and when they spend their EPiQS funding, without intensive oversight by program managers. This also adds a premium on the value of each EPiQS award.
- Quantum materials researchers, including both EPiQS grantees and non-grantees and the expert panel, agree that EPiQS has focused its funding on the most accomplished researchers in this field, each with a record of important scientific achievements. Thus, EPiQS also concentrates its funding on researchers experienced in managing research teams and in producing substantive discoveries, providing additional leverage.

With those factors in mind, the EPiQS investment averaging \$18 million per year can have a significant influence on the U.S. research community in quantum materials. On an individual

basis, self-reported figures from grantees show that for most awardees, the support from their EPiQS awards accounts for no more than half of the annual budgets for their research teams (see **Figure 2-1**). (It is unknown how the grantees factored in the different indirect cost rates for EPiQS versus federal awards, if at all.)

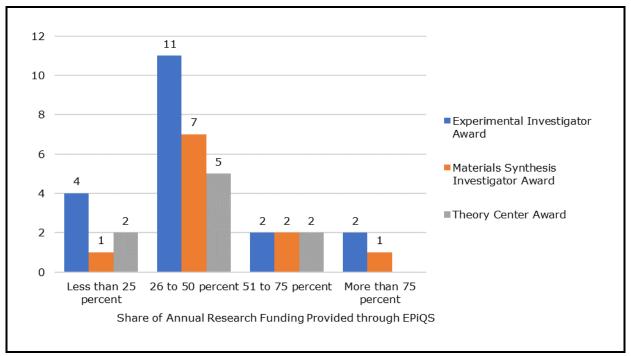


Figure 2-1. EPiQS Funding as a Share of Each Awardee's Annual Research Budget, by Award Type

Thus, on a per-investigator basis, EPiQS funding is substantial and potentially transformative to each researcher's efforts, but none of the awardees have become entirely dependent on EPiQS support.

## 2.3 Assessing the Self-Assessment of EPiQS: Key Challenges in Indicator Development

The RTI team was asked to evaluate the foundation's "Indicators and Metrics Framework" for measuring the progress of EPiQS, developed as part of its 2015 Strategic Review. After reviewing the metrics intended for use during the timeframe of this evaluation (2015 to 2018), as shown in **Table 2-1**, we encountered difficulties in interpreting the metrics in a manner that team members could operationalize. Although the metrics presented are quantitative, in that each one is expressed as a number, some require subjective judgments to generate corresponding values.

For example, one metric is a count of the "number of new methods, techniques, models and instruments developed" based on EPiQS funds. Previous research on the topic of measuring scientific advancement reveals that there can be substantial disagreement, even among scientists in the same research specialization, over what is a discrete method versus a technique, and even whether a particular method is truly "new" or instead a derivative of an earlier development. Although grantees include details of their discoveries and accomplishments in their annual grantee reports, expert opinion is needed to identify which accomplishments should be labeled as a method or technique, determine if the accomplishment qualifies as "new," and how to track consistently the exact number of new developments reported by each grantee. It could be helpful, as a starting point, if the EPiQS program staff extracted and compiled an annual inventory of these developments using the grantee reports, so that it could be evaluated by outside experts. For example, the international expert panel generated a description of key achievements in guantum matter research since 2013, grouped by topical area, and indicated which EPiQS awardees were primarily responsible for each achievement. The expert panel report could be annotated by the EPiQS program staff and compared to the items listed by grantees in the "Scientific Advances" section of their annual reports. This would provide some independent validation of the number of advances reported that can be counted under this metric.

Outcome	Metric(s)
EPiQS grantees have developed new methods, techniques, models, and instruments.	Number of new methods, techniques, models, and instruments developed under EPiQS funding
EPiQS grantees have made advances in knowledge of theoretical approaches, materials synthesis, and experimentation.	<ul> <li>Number of grantees who have made significant advances based on EPiQS team review and other appropriate expert evaluation, and as indicated by</li> <li>Number of publications and presentations on newly developed methods, techniques, models, and instruments</li> <li>Number of projects, publications, and presentations coauthored by a visiting scholar or postdoc supported through a Theory Center award</li> <li>Number of publications and presentations resulting from EPiQS-stimulated collaborations</li> <li>Number of citations of these publications and presentations</li> </ul>
A target set of leading institutions have enhanced their capability to synthesize novel quantum materials through increased faculty expertise.	Number of EPiQS-endorsed synthesis experts who are hired at target institutions

 Table 2-1.
 EPiQS Metrics for Intermediate Term Impacts (2015–2018)

Source: FINAL EPiQS Strategy Review Appendix II—Indicator and Metrics Framework<sup>8</sup>

<sup>&</sup>lt;sup>8</sup> Gordon and Betty Moore Foundation. (2015). *Final EPiQS Strategy Review Appendix II: Indicators and Metrics Framework*. Palo Alto, CA: Gordon and Betty Moore Foundation.

Although the EPiQS program staff very appropriately instruct the awardees that they are not evaluating research performance by crude metrics such as publication counts and number of citations, the metrics that attempt to measure the advances achieved by grantees include counts of publications and citations. There is extensive discussion in the scientific literature as to how these types of metrics are unreliable tools for measuring research productivity, quality, or impact.<sup>9</sup> As an example, citations counts are very time-dependent, so that a publication now deemed as a seminal work may have taken years to accumulate a significant number of citations. The scientometric analysis performed in this evaluation contains some examples of citation-based metrics to describe effects attributable to EPiQS funding.

Tracking the number of synthesis researchers hired in a given time period is a helpful indicator. However, it is difficult to attribute any individual hiring decision to the influence of EPiQS. These decisions are affected by many confounding variables outside of the control of EPiQS. One such factor is the interest in condensed matter physics shown by the department's faculty focused in other topics, as hires are influenced by departmental consensus, not simply the judgment of the faculty members in one area.

Our recommendation is to design a metrics framework that maps more directly to the EPiQS Theory of Change. Is it possible to validate that EPiQS synthesists are developing novel material samples, and how widely are those samples being shared? What new types of equipment are EPiQS investigators able to purchase and use (not only develop) with their funding? Are investigators taking advantage of the freedom and discretion to pursue new research goals?

Some of these metrics can be derived from grantee reports. However, some metrics should use sources other than self-reported data to help ensure validity. For example, the EPiQS program staff has used the accounts of new research collaborations listed in grantee reports to illustrate the number, nature, and participants involved in collaborations among grantees. This addresses directly the ability of EPiQS to facilitate the development of a more cohesive and interactive research community. The inventory of collaborations can also indicate which collaborations were based on the distribution of sample materials, another key objective. These reports can then be compared to data on the number and nature of papers whose coauthors include more than one EPiQS awardee, providing an external data source for analyzing the self-reported data.

<sup>&</sup>lt;sup>9</sup> A summary of some issues is found in Hicks, D., Wouters, P., Waltman, L., de Rijcke, S. and Rafols, I. (2015). The Leiden Manifesto for research metrics. *Nature*, **520**, 429–431.

We do feel that there are some new techniques for analyzing scientific publications that might be applicable to the metrics in the existing framework. For example, a machine learning based technique of analyzing documents, called topic modeling, can be used to identify trends and concepts that appear in the literature, and then traced over time to understand impact.<sup>10</sup> We note that many of these techniques are still exploratory in nature, and should be used cautiously.

Our recommendation is that developing a metrics framework may be a helpful undertaking, provided that (a) the indicators provide meaningful information about trends and activities important to EPiQS, and (b) changes in the indicators could prompt changes or adjustments in program management (see box, **Guidance in Formulating Progress Metrics**). For

example, if the number of scientific advances produced by EPiOS awardees declines from

#### Guidance in Formulating Progress Metrics

The RTI team recommends following these principles in developing a metrics framework for EPiQS.

**Relevance:** Does the metric measure key elements of the Theory of Change? Indicators could monitor whether or not the stature of grantees is growing (evidenced by invited talks or prominent roles in conferences), or access to materials and probes (tracking equipment purchases, transfers of materials, visits to user facilities), and collaborations (co-authored articles or other joint efforts).

**Utility:** Can EPiQS staff take action based on trends in the metrics? If the rate of collaboration seems to be lagging, as an example, the Investigator Symposium could be restructured to provide more time for discussions among grantees.

**Attribution:** Metrics should primarily focus on trends that can be attributed directly to the influence of EPiQS. Metrics with more tenuous attribution, such as national trends in faculty hiring, should be included with a strong caveat that the trend may not be influenced by the results of EPiQS.

**Consistency:** Rather than using different metrics for each time period, monitor a single set of metrics, while understanding that some metrics change over a longer time horizon than others.

year to year, is this significant? Or is the total number of advances achieved in a time period sufficiently informative? In general, metrics are more useful when they are designed and selected using a principled approach, where the rationale for how EPiQS is intended to achieve results determines what is monitored.

<sup>&</sup>lt;sup>10</sup> See for example, Gerow A., Hu Y., Boyd-Graber J., Blei D.M., and Evans J.A. (2018). Measuring discursive influence across scholarship. *Proceedings of the National Academy of Science*, published 12 March at Mar 2018, 201719792; DOI: 10.1073/pnas.1719792115.

## 3. IMPLEMENTATION OF EPiQS: INNOVATIONS IN PROGRAM DESIGN & MANAGEMENT

Given the rationale for the design of the EPiQS in its Theory of Change, how well did implementation of the initiative reflect that rationale and conform to the design parameters? This component of the evaluation was informed primarily by discussions with the grantees themselves, as well as reviewers involved in the awardee selection process, and program documentation that records decisions and actions undertaken by program staff.

#### Key Findings

- The competition and selection process for Investigator awards elicited proposals that are very different from research likely to be funded by federal sources and represent the most compelling research visions and ideas of recognized leaders in the field.
- Management of the EPiQS program fulfilled the objective of providing researchers with the resources and freedom to innovate, and program staff were integral to that achievement.
- New modes for communicating the program's design and goals to grantees and other stakeholders may help shape expectations and perceptions.

## 3.1 Awardee Selection: Eliciting the Best Ideas from Top Scientists

As an integrated program of awards with several distinct purposes and selection criteria, EPiQS represents a novel approach to funding physical sciences research. For its Investigator awards, EPiQS varies from the approach of most federal agencies in that it primarily funds "people, not projects," in the parlance of the Howard Hughes Medical Institute (which has a similar philosophy). Expert reviewers were employed to rate the proposals received, especially for the Experimental Investigator and Synthesis Investigator competitions. Unlike a more traditional federal peer review process, reviewers were instructed to weigh heavily the investigator's research accomplishments over the past 8 to 10 years in evaluating each proposal, in addition to the quality of the idea in the proposal. According to reviewers, it was very clear that EPiQS intended to support investigators who had already proven that they could produce important new discoveries by employing innovative approaches.

There is no evidence that this "people-centered" approach to selecting grantees has been used in any previous research program in the physical sciences. In most federal programs, with the exception of some young investigator awards, applications are evaluated based on the research idea proposed and then secondarily on whether the applicant has the skills and resources to carry out that idea (where past achievements may or may not be used as an indicator). The experience of the foundation's Marine Microbiology Initiative, along with the similar design used in the Howard Hughes Medical Institute Fellows program, provided evidence that the investigator-focused award approach has merit if properly adapted to the specific circumstances of a given field. Therefore, the awardee selection approach implemented by EPiQS is an experiment with a credible empirical basis.

Applicants for EPiQS funding (both successful and unsuccessful) commented that the proposal template was also very unusual, in comparison to standard federal funding applications. The proposals had to be relatively short and could not contain figures or references. By limiting the space available to write but also emphasizing that proposals should present bold ideas, the template challenged applicants to think about their research plans in a more creative way. In the grantee survey, half of Equipment grantees and 100% of Experimental Investigator and Materials Synthesis Investigator grantees (including Moore Fellows in Materials Synthesis) indicated that their proposed research topic and agenda outlined in their EPiQS proposal differed in substance from a typical proposal they would submit to a federal agency. Significantly, several applicants commented that producing a *shorter* proposal required much *more* time on their part, to think through their research plan more clearly and to convey a compelling vision more concisely.

A few senior researchers cautioned during interviews that there is a potential weakness to this approach, in that an applicant with a great idea, but who is not very skilled at expressing it, might be passed over in favor of a candidate with a more 'polished' presentation (on paper). This approach may also favor more senior researchers, as they have much more experience in how to write proposals well, both in generating successful proposals and in serving as reviewers. However, the EPiQS selection process required evidence that each candidate was successful at performing ambitious research, and not simply describing it. It is unlikely that this feature of the approach compromised the validity of the awardee selection.

## 3.2 Enabling Flexibility through Program Oversight: Impact on Innovation

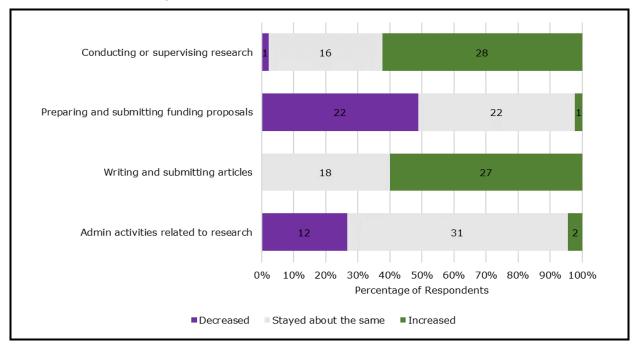
During interviews, grantees confirmed that they were afforded the "freedom to innovate" within the structure of the EPiQS funding, and most took productive advantage of that freedom. This freedom was interpreted by grantees as a signal that the EPiQS program staff trusted them to make the best decisions about how to conduct their own research, and that they should use their own judgment without fear of being "second-guessed" by program managers.

This trust was evident to grantees starting with the post-award negotiation. One grantee exclaimed that the attitude of EPiQS was "surprisingly humane." In a typical funding opportunity, the applicant makes an educated guess about the amount of funding that is reasonable to request, and then engages in bargaining with the funder to revise the scope of the proposal to fit the actual award amount. The EPiQS Investigators were told the award up-front, and simply had to design a research plan that fit the fixed budget.

Grantees expressed the common sentiment that the management and administration of the EPiQS funding were streamlined and straightforward. For example, grantees feel the reporting requirements attached to the EPiQS awards are less burdensome than any federal grant. Grantees complete a relatively short annual summary of their work. During the year, they can use the funds to make purchases, hire postdocs, and travel to conferences, and at most the only "process" was a quick call to an EPiQS program manager to affirm consent to that decision. This approach stands in stark contrast to typical approval processes for expenditures involving federal grant funding. For example, NSF grants require proposers to budget for conference travel in advance, and obtain specific permission for overseas travel. While it may seem that EPiQS is comparatively lax in enforcing accountability over spending, we note that the initiative provides guidance on allowable expenses, and grantee institutions submit annual financial reports that are audited by the foundation.

Due to the relatively little time and effort involved in administrative matters, EPiQS awardees could be more focused on their research activities and interests. As shown in **Figure 3-1**, researchers also devoted more time to mentoring junior researchers and to preparing articles for submission. Some awardees noted that the EPiQS funding enabled them to spend more time in their laboratory working alongside their graduate students and postdocs, rather than sitting in their offices completing paperwork. The investigators were therefore more directly accessible to their research team members. Those students and postdocs could also receive training directly from the PI on how to use laboratory equipment and instruments. By observing the PI at work in the lab, these junior researchers benefited from "on the job" learning about the research process.

Similarly, grantees felt that this additional time afforded them more opportunities to think deeply about their research, formulate hypotheses, and analyze results. One researcher noted that the EPiQS funding allowed him to hire a postdoc who could take responsibility for managing day-to-day activities in the laboratory. This gave the researcher the opportunity to work at home and focus intensively on writing articles about notable research results, and decide on future research directions. In general, grantees interviewed felt that the time gained by reducing their administrative burden helped them to produce higher quality articles and more compelling research proposals to other funders.



# Figure 3-1. Comparison of the Allocation of Researcher Time Across Activities, before and after EPiQS Award

Grantees (and representatives of the grantees' institutions who handle funding matters) uniformly reported that interactions with Moore Foundation staff were pleasant, cordial, and productive. Other stakeholders who met with the EPiQS program staff, such as departmental chairs and federal program managers, commented that EPiQS was led by managers who were extremely knowledgeable about the field, highly interested in the work conducted by awardees, and responsive to inquiries and concerns. This provided additional reassurance to grantees in particular they could interact with the EPiQS staff as peers, not as supervisors. Several grantees noted that feedback from EPiQS program managers in some cases provided valuable new ideas to investigate. Almost all grantees felt that the EPiQS program staff had established an interpersonal dynamic such that they felt equally comfortable asking the staff for specific programmatic guidance or using them as a "sounding board" for new research ideas.

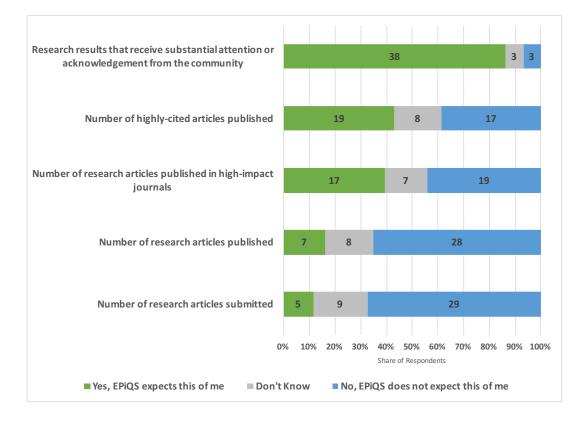
## 3.3 Addressing Potential Ambiguity in Program Communications

During interviews, some grantees (fewer than ten of the approximately 40 grantees interviewed) expressed slight apprehension that as their current funding awards approached their end, they had only a vague idea of what the foundation expected them to show from their research. One investigator stated bluntly, "I imagine that I have to show *something* for

the \$1.8 million that they gave me." While not a major concern, there may be some opportunity to consider how program expectations are communicated to grantees.

The challenge to the EPiQS program managers is that in any funding program, communication is constantly subject to misinterpretation. We note that grantees felt that the EPiQS program managers were always prompt in returning calls and e-mails if the grantees had questions. A few of the grantees who were unsure about the issue of expectations did reach out to the program managers, and reported that the resulting discussions were very constructive.

The EPiQS program staff has been very effective in informing grantees that the quality of their research results will not be evaluated with simplistic metrics such as citation impact measures, or counts of publications in high-impact journals. As shown below in Error! Reference source not found., a number of grantees still believe that EPiQS expects them to produce some quantity of highly-cited articles or articles appearing in high-impact journals. In the absence of more specific guidance, such grantees may default to metrics that are imposed by other sponsors. One way to address this might be to shift that perception away from "expectations"—what EPiQS wants from grantees—and move towards discussing "aspirations"—the varieties of achievements and results that the initiative intended to enable. Grantees could be reassured to know that EPiQS is more focused on ensuring that grantees are being sufficiently ambitious in their efforts, regardless of whether that leads to articles or citations.



#### Figure 3-2: Grantee Perceptions of Metrics Expected to Fulfill Under EPiQS Funding

Ultimately, the EPiQS Initiative has a very ambitious goal: to "catalyze transformative change in the science of emergent phenomena in quantum materials." As noted previously, the term "transformative change" is very subjective and open to broad interpretation. During interviews with grantees, it became clear that the concerns over the "expectations" placed on EPiQS grantees stemmed from that ambiguity. As the current set of grants reach the end of their funding period, the program staff could spend some time discussing what they consider to be "transformative change" in more concrete terms, and how they believe awardees may be contributing to potentially transformative research through both their achievements and their failures. A few grantees pointed out that the EPiQS grantee reports include a section where grantees should report their failures, which is a very unusual feature compared to grant reports required by other sponsors. If appropriate, the staff could also discuss how they use discussions about research failures positive and constructive information, as failures are a necessary byproduct of high-risk research.

## 4. ACCELERATING AND TRANSFORMING RESEARCH: THE IMPACT OF EPiQS ON GRANTEES

The funds awarded by EPiQS are considerable, and these grants have had a range of effects on the grantees—in some cases, dramatic effects. At least one grantee felt that his scientific career would have been mostly over by now, but for his EPiQS award. For some other grantees, the EPiQS award provides a comfortable budget on top of their existing federal funding to expand their prior investigations in new directions. In summary, all grantees experienced significant gains in their ability to pursue ambitious and promising new research findings.

#### **Key Findings**

- EPiQS grantees used their funding to hire researchers and acquire new equipment. Those inputs to their research efforts will benefit grantees beyond the EPiQS award period.
- EPiQS has enabled grantees to be more dynamic in their research, and to pursue more ambitious research objectives with unconventional approaches. As one consequence, this work helped grantees achieve results that contributed to follow-on funding awards.
- Grantees have gained new opportunities to form productive research collaborations, and they are intensifying collaborations and exchanges within and beyond the EPiQS community.

### 4.1 Investments in Research Inputs—Human and Physical

The two most immediate ways that EPiQS changed the trajectories of its grantees' research are instances where PIs hired new postdocs and when they acquired new equipment. **Figure 4-1** displays the survey responses on various ways that grantees used their funding. This figure excludes the Theory Center grants (where all funds went to hiring postdoctoral researchers and to host visiting scientists) and the Equipment Development grants (where the funds specifically support equipment purchases and development).

The most common uses of funding were for personnel-related charges. Essentially all grantees hired a new postdoctoral researcher, and also used EPiQS funds to support graduate students working in the laboratories. By expanding the size of their research teams, EPiQS PIs could take on more ambitious research plans (see **Section 4.2** below). This also had a direct and beneficial impact on the postdocs themselves, as explored further in **Section 7**. Grantees reported during interviews that while federal funds help to support some postdocs in their labs, the flexibility of the EPiQS funding meant that they could take the risk of hiring a postdoc with a somewhat different background than usual, to help the

grantee explore new ideas and learn a new domain. For example, one Experimental Investigator hired a postdoc with a Ph.D. in Chemistry rather than Physics. That postdoc's expertise helped the grantee to understand better some key aspects of materials synthesis that played a key role in developing a new approach to analyzing quantum materials. That sort of "unconventional" hire might be difficult under a federal grant, where a PI must show that any postdoc hired has training directly related to the funded research project.

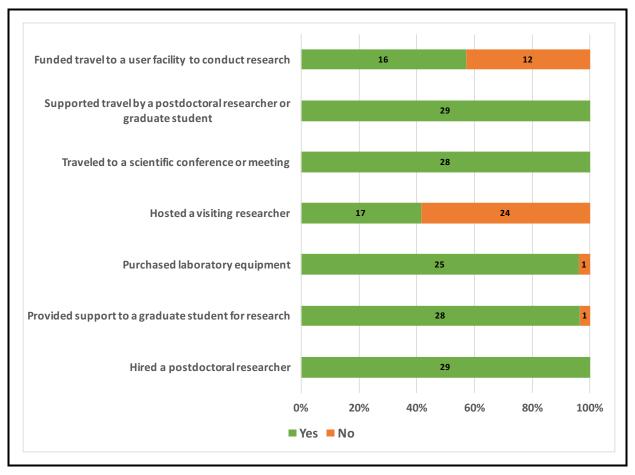


Figure 4-1. Spending Allocations Made by Grantees with EPiQS Funding

Travel was a second area of investment, mostly for conference travel or to cover the expenses of hosting visiting scientists. Federal grants generally provide limited funds for travel, and there may be significant administrative approvals involved (particularly to attend international conferences). By providing flexible funds for travel, EPiQS enables its grantees and their associated postdocs and graduate students to communicate their research results directly to peers, and to gain new opportunities to meet potential research collaborators.

Another important use of funds is to cover travel and related expenses for traveling to major scientific user facilities that offer unique instruments for materials characterization and measurement. More than half of Investigator grantees surveyed used EPiQS funds to

support such travel. These facilities, which are generally supported by the DOE, are often in high demand. For example, the Advanced Neutron Source at Argonne National Laboratory hosts over 2,000 users per year. Grantees report that due to the long lead times required to reserve time at a user facility, aligning their time slot to use a facility and their federal funding cycle is challenging. Grantees used the flexibility of the EPiQS funds to make sure that they had resources to travel to a user facility exactly when needed.

Finally, grantees discussed in interviews how they used their EPiQS funds to purchase significant new instruments or other pieces of equipment. In some cases, the items purchased were needed to take their research in a new direction. In others, they were simply to update or replace existing equipment that had become outdated. Accounting for equipment purchases using federal funding can be cumbersome and time-consuming, and so the flexibility of the EPiQS funding provided a very helpful mechanism for upgrading a grantee's own laboratory. This use of funding directly supports the objective of providing researchers with access to state-of-the-art instrumentation and probes, at a lower scale than the development of a major new facility.

One grantee noted in particular that technical advances in scientific instrumentation meant that the equipment that could be purchased today for a single laboratory offers capabilities far beyond what was affordable five years ago. Furthermore, the expert panel's report points out a number of cases where grantees have used EPiQS funding to take off-the-shelf instruments and equipment and improve their capabilities, or to combine different probes in novel configurations to make ground-breaking empirical observations. The longer-term implications of this are discussed in **Section 6**.

## 4.2 Effect of "Freedom to Innovate" on Research Risks and Results

The proposal process for EPiQS Investigators encouraged them to submit ideas for "highrisk, high-reward" research. This concept of risk was discussed extensively in grantee interviews. When these researchers say that they are pursuing "risky" research, they often mean that it presents a challenge to their own abilities. Roughly half of the grantees interviewed framed risky research as an investigation that takes them into domains where they have little experience or expertise, or where they believe that they will be successful but face great uncertainty of how or when they'll succeed. A large portion of the grantees interviewed supported the notion that research failures were a positive indicator that they were attempting investigations and research approaches that were truly risky, rather than being conservative.

In these discussions, grantees routinely stated that such research would be almost impossible to fund with federal research support, because proposal reviewers are predisposed to reject PIs who take such risks. While EPiQS selected awardees based on a record of accomplishments, peer review panels tend to look more narrowly at a PI's training and research focus. A PI who strays from those familiar domains will be told that essentially, they should stick to what they know and not try to move into new territory. A more detailed analysis of each grantee's past and current work could reveal information on the degree to which particular grantees had used EPiQS funding to move beyond their "comfort zone" of familiar science.

Some of the examples cited by the expert panel provide evidence that grantees have attempted and executed investigations beyond those possible with more modest and restrictive federal grants. For example, the panel notes that

*EPiQS has given new impetus to an enduring grand challenge in quantum materials research—the origin of high temperature superconductivity in layered cuprates ... Funding for research in this field has been difficult to obtain from government-funded programs, which are often driven by short-term trends.*<sup>11</sup>

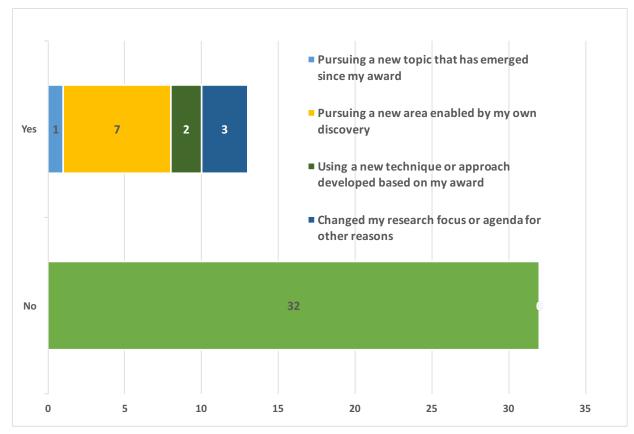
The panel cites work by grantees S. Davis, L. Taillefer, and N.P. Ong as representative of important new results in this area enabled directly by EPiQS. The panel also highlighted that EPiQS funds enabled grantee N. Gedik at MIT to "optimize a wide variety of instruments" to measure non-equilibrium phenomena as they emerge in quantum materials in his own laboratory.

At a personal level, grantees discussed ways in which the nature of EPiQS funding freed them to take new approaches to existing research questions, or to engage in deeper study of unfamiliar topics to inform their research. One commonly-cited activity was the degree to which Experimental Investigators are training themselves on techniques in materials synthesis, so that they are not entirely dependent on other researchers for sample materials. The process of learning synthesis also provided researchers with new insights that contributed to their empirical work. At MIT, for example, Profs. Jarillo-Herrero, Gedik and his colleagues frequently consult with Prof. Joe Chekelsky, a Moore Fellow in Materials Synthesis, on synthesizing crystals. Prof. Jarillo-Herrero purchased a glove box and other equipment that enabled him to build off of his expertise in graphene to synthesize and investigate other types of two-dimensional materials. This capability is likely to have contributed to two recent notable discoveries involving his lab—the observation of magnetism in a monolayer composed of CrI3, and the manipulation of layers of graphene to induce superconductivity.<sup>12</sup>

<sup>&</sup>lt;sup>11</sup> Keimer, B. et al. (2018). "Emergent Phenomena in Quantum Systems: Expert Panel Report." Unpublished report prepared for the Gordon and Betty Moore Foundation, February 20, 2018, at p. 6. <sup>12</sup> Huang, B. et al. (2017). Layer-dependent ferromagnetism in a van der Waals crystal down to the monolayer limit. *Nature*, **546**, 270–273; Gibney, E. (2018). Surprise graphene discovery could unlock secrets of superconductivity. *Nature*, **555**, 151–152.

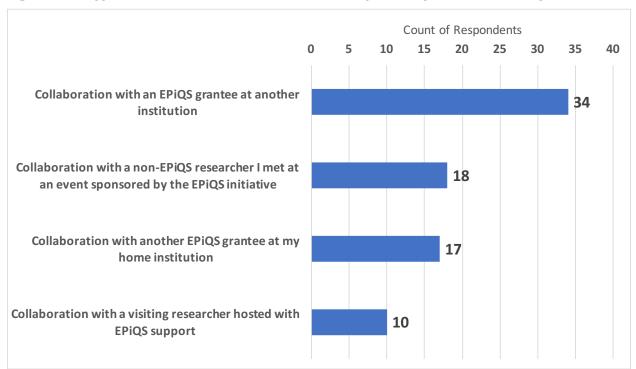
The survey of grantees also asked respondents to estimate whether or not they took advantage of the EPiQS policy that allows grantees to shift research away from their original proposed topic. **Figure 4-2** shows that of the grantees responding to the survey, less than a third feel that their research direction today is substantially different from what they had proposed. Of those, most were now pursuing topics uncovered by discoveries that they had made in the course of their research after award. While not all grantees took advantage of the freedom to shift their research, interviews reflect that for some researchers, this was an important feature of the EPiQS funding.





# 4.3 Collaboration Patterns among EPiQS PIs

A substantial majority of grantees responding to our survey indicated that they had started a new research collaboration attributable at least in part to their EPiQS funding. 44 of the 46 grantees responding to the survey reported at least one new research collaboration. All but one grantee felt that the EPiQS initiative played a role in forming new collaborations. Of those, most stated that at least one collaboration involved another EPiQS grantee, as shown in **Figure 4-3**. 18 reported that participation in an EPiQS-sponsored activity (including meetings and conferences sponsored by EPiQS that were open to nongrantee researchers) contributed to at least one new collaboration. This provides some view into how EPiQS funding is able to influence the work of researchers beyond the immediate pool of grantees.



## Figure 4-3: Types of New Research Collaborations Reported by Grantees Surveyed

Note: Respondents were allowed to select more than one answer

Key among the mechanisms that have created new opportunities to collaborate and that have ultimately led to new collaborations is the Investigator Symposium. Grantees described this venue as an environment ripe for information-rich interactions among PIs who may not otherwise have opportunities for comparable exchanges at a larger scale event or an event with a focus diluted by topics outside of quantum materials.

An indirect but notable mechanism by which EPiQS affords awardees greater opportunities to collaborate is the prestige and recognition associated with the awards themselves. Virtually all PIs (other than Theory Center PIs) surveyed for the evaluation agreed with the statement that their EPiQS awards increase their recognition or stature among their peers, and nearly two-thirds reported that the increase was significant. The prevalence of sentiment was uniform for PIs across all career stages. During interviews, PIs who were in the earlier stages of their careers or who come from demographic groups typically under-represented in physics faculties (e.g., females) stated that this recognition had a substantial impact on their patterns of collaboration. These individuals felt that the EPiQS award had validated their status as accomplished researchers in quantum materials. They reported the feeling that after receiving their awards, they were taken more seriously by other EPiQS awardees, non-EPiQS quantum materials researchers, and even by their faculty peers from other subdisciplines of physics. As a result, they found it easier to approach peer scientists whom they wanted to meet and explore potential joint research, and they felt that those peers accepted their invitations to collaborate more readily. This offers some support for the view that an EPiQS award has a disproportionate impact on researchers who are more junior or less prolific in the field, and that EPiQS played an important role in enabling those researchers to contribute their ideas to discussions and cooperative efforts involving more established researchers.

Postdocs represented another prominent mechanism through which new collaborations occurred. Both the directly funded Moore Postdoctoral Scholars and the synthesis and experimental postdocs hired at the discretion of the Investigators were often active across different labs. This activity forged new lines of communication, which has led in some cases to formal collaborations and in other cases of informal collaborations that nonetheless have served to increase the quality of ideas circulating among grantees, postdocs, and some non-grantees, as well. For example, when postdocs begin in their EPiQS-supported positions, they bring their existing connections to their former collaborators and mentors, which sometimes lead to formal connections between groups upon their arrival.

# **5. INSTITUTIONAL IMPACTS OF EPiQS**

The EPiQS awards are investments in the grantees' host institutions as well as investments in those individual researchers. In several cases, those institutions are co-investing with the EPiQS Initiatives on awards, particularly for Theory Centers and equipment grants. There is nascent evidence that EPiQS has changed the strategic behaviors of key U.S. universities so that they are prioritizing investments in quantum materials research, especially in synthesis.

## **Key Findings**

- EPiQS funding contributed to the creation of positions in materials synthesis for the Moore Fellows in Materials Synthesis, and appears to be encouraging broader hiring prospects for researchers in synthesis.
- Institutions that house multiple grantees funded through different EPiQS strategies experienced some synergistic benefits from intra-institutional collaborations, but institutional cultures may impede this.
- By creating new postdoctoral positions through Theory Center awards and through funding to Investigators, EPiQS expanded the range of research undertaken at those institutions and provided benefits to faculty beyond the direct awardees.

## **5.1 EPiQS as a Factor in the Growing Market for Materials Synthesis** Faculty

One specific objective of the EPiQS synthesis funding strategy is to increase the stature and appreciation of materials synthesis experts in the U.S. quantum research community. Ideally, this increased stature would then provide an incentive for U.S. universities to create more faculty positions in this area, which would both expand and deepen the pool of institutions that can support U.S. research competitiveness in this critical area.

Faculty hiring might be expected to be a lagging indicator of impact from EPiQS. The hiring process for a new faculty member can take well over a year from the first planning through the interview process to a final hiring decision. Also, it is important to realize that hiring decisions are made by committee. For a physics department to hire a new faculty member in quantum materials research, faculty specializing in astrophysics, high energy physics, and any other subdiscipline represented at that department must support that action. This fact complicates efforts by the EPiQS Initiative to influence hiring decisions.

Even so, there are signs that EPiQS is already shifting the job market in this area, especially for materials synthesis. At the time of this study, two Moore Fellows in Materials Synthesis had received awards—Profs. James Analytis at UC Berkeley, and Joe Checkelesky at MIT. These two awards conferred particular benefits to these early-career researchers. Representatives of their respective institutions confirmed that both the prestige of the award as well as the award funding strengthened departmental support for hiring these individuals into new tenure-track faculty positions. These representatives noted in particular that their institutions were able to arrange for more desirable laboratory space, and invest more institutional resources into building out that space, due to the availability of funding from EPiQS. Quantum materials researchers at other institutions also looked at hiring the awardees of Moore Fellowships in Materials Synthesis, and this appears to be a key factor in the recent appointment of Prof. Julia Mundy to the faculty of the Physics Department at Harvard University (see **box**). By helping to facilitate the hiring of new faculty in materials synthesis at major research universities, EPiQS expands the pool of talented researchers in this field and provides new role models for young researchers who are interested in pursuing synthesis as a research specialization.

#### Case Study in Materials Synthesis Hiring: Prof. Julia Mundy at Harvard

Dr. Julia Mundy was named a Moore Fellow in Materials Synthesis after the period of this evaluation study. Her experience provides an instructive example of the influence of EPiQS in the dynamics of the labor market for materials synthesists.

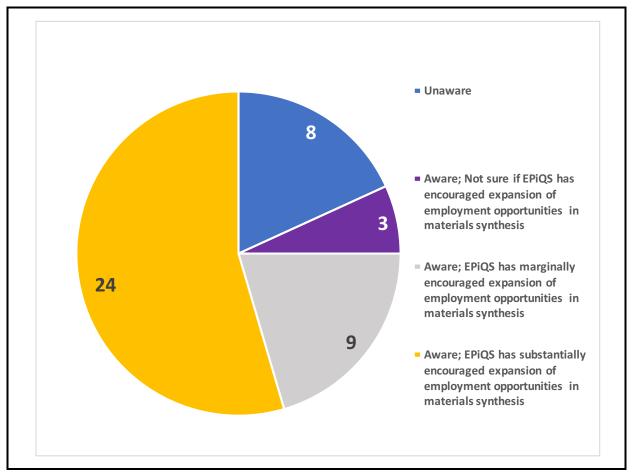
Prof. Mundy's connections to the EPiQS community of researchers dates back to her work as a Graduate Research Fellow at Cornell University under Prof. Darrell Schlom, a current Equipment Development awardee. After earning her Ph.D. in May 2014, she spent a year on a fellowship with the American Association for the Advancement of Science, and in 2015 became a UC President's Postdoctoral Fellow at UC Berkeley where she began working with Prof. Ramamoorthy Ramesh. About one year into her two and one-half year postdoc, Ramesh was awarded a Rapid Response grant from EPiQS, which enabled his research group to seize timely opportunities in new areas that ultimately yielded a flurry of results.

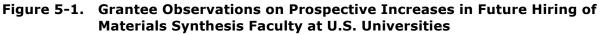
In early 2018, Prof. Mundy was named a Moore Fellow in Materials Synthesis, and received an appointment on the faculty of the Physics Department of Harvard University. Significantly, she is the first faculty member hired in recent memory specializing in synthesis. Discussions with Harvard faculty members and institutional representatives revealed that the department had been considering a new faculty hire in this specialization for a few years. They had encountered problems in finding the right candidate and overcoming institutional barriers to hiring a synthesist, such as the cost of providing an appropriate laboratory for materials synthesis. Prof. Mundy's record of work with current EPiQS grantees, and the prestige and funding associated with her own award, appears to have tipped the scales and facilitated Harvard's decision to add a materials synthesis expert to its faculty.

At several institutions housing multiple EPiQS grantees, institutional representatives revealed that they do have plans to hire more faculty focused on quantum materials, including some who focus on materials synthesis. Those discussions showed, however, that these institutions had decided to make a strategic investment in condensed matter physics even before the EPiQS Initiative was announced. Obviously, the additional resources devoted to quantum materials have garnered active interest from universities, and interviewees noted anecdotally that they are seeing more position announcements for faculty slots in this domain.

EPiQS grantees also reported that other institutions are increasing hiring in this area. A majority of respondents to the grantee survey indicated that there was at least some movement to hire new quantum materials faculty at their institutions and that EPiQS played some kind of role in that decision (see **Figure 5-1**). Grantees and non-grantees interviewed on this topic reported that they see more position announcements in physics departments that solicit applications from materials synthesis researchers. They also have had informal

discussions at conferences and other gatherings with colleagues from different universities that included mentions that a number of departments have started to seek approval to create a new faculty position in materials synthesis. If valid, the trends relayed in such anecdotes should be reflected in future public position announcements and faculty recruitment efforts. Monitoring academic job boards, such as HigherEdJobs.com, may yield more substantial evidence of hiring in materials synthesis. However, most faculty position announcements in areas such as experimental condensed matter physics do not specify details such as experience in synthesis as criteria, so such monitoring would need to be supplemented by conversations with faculty in the field.





## 5.2 Multi-grantee versus Single-Grantee Institutions: Potential Synergies

As noted in earlier sections, quantum materials research is expected to benefit from the increased linkages between theory, experimentation, and synthesis. As one test of that

hypothesis, we examined collaboration patterns at institutions with awardees spanning the related EPiOS funding strategies: Theory Centers, Experimental Investigators, Materials Synthesis Investigators, and Moore Fellows in Materials Synthesis. In institutions housing multiple EPiQS grantees, awardees confirmed in general through survey responses that they interact more with the other awardees at their same institutions than before EPiOS (see Figure 5-2). Interviews and site visits revealed that the level of interaction varied dramatically. For example, some universities seemed particularly successful at encouraging collaboration and interaction among grantees in synthesis and experimentation, as well as theory centers (if present). At other institutions, the interaction has been somewhat superficial. The interviews revealed that the level of interaction depends heavily on the institutional culture at that university. At one institution, faculty by tradition leave their office doors open when working to welcome colleagues and students who want to stop by and talk. There are frequent colloquia attended by multiple faculty, and the office design has numerous spaces for informal collaboration. As a result, this institution showed indications that both informal and formal collaborations among awardees are common, and that graduate students and postdocs working with different EPiQS grantees were likely to have their own joint discussions and social gatherings. At another institution, faculty members commented that researchers were unaccustomed to walking around and talking informally to others, and that a typical faculty member would almost never walk even to a neighboring building to visit a colleague, reducing the instances of spontaneous discussion. The grantees at this institution admitted that they had encountered problems in trying to arrange discussions with other grantees at that institution.

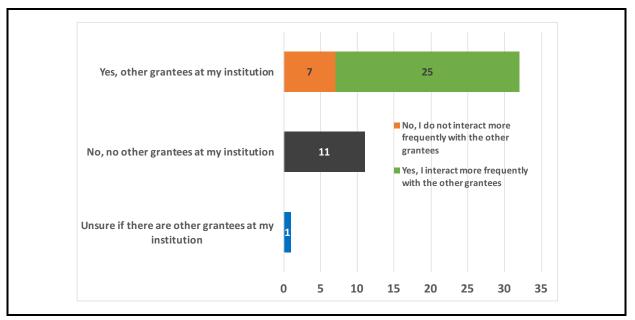


Figure 5-2. Degree of Interaction at Multi-grantee Institutions

We note that some institutions are making a concerted effort to use EPiQS funding as a tool for "cluster hires," where they are investing not only in supporting their grantees but also hiring new faculty in quantum materials and even recruiting other EPiQS grantees. The one clear example of this is Rutgers University, which has increased its stature in quantum materials research by hiring Prof. Jak Chakalian from University of Arkansas (an Experimental Investigator) and forming a partnership with the faculty at Princeton to encourage joint work in quantum materials (**see box**).

The role of postdoctoral researchers and graduate students should be noted on this point. In many cases, interviewees (both postdocs and faculty) stated that while faculty-to-faculty interactions were less common, there were many more cases where postdocs from one lab talked to a faculty member in a different lab or where postdocs and graduate students from two different labs got together to discuss theory and research. While the Theory of

#### **Quantum Materials at Rutgers**

Recent developments at Rutgers since the start of the initiative reflect an effort to leverage funding from EPiQS to build the institution's visibility and reputation in quantum materials. Initially, in 2014, Materials Synthesis Investigator awards were granted to Sang-Wook Cheong and Seongshik Oh, two highly-accomplished synthesis faculty with ambitious goals. Prior to EPiQS, these faculty members had helped launch the Rutgers Center for Emergent Materials with support from the University.

Under the leadership of Cheong, the center's director, capacity for quantum materials research continued growing. Rutgers leveraged two EPiOS contributions (one in 2015 and the other in 2016), to host a highly-regarded Symposium on Quantum Materials Synthesis in 2016. Coinciding with the planning of these activities, the department strategically hired Prof. Jak Chakhalian who added valuable new expertise. Chakhalian was also an EPiQS Experimental Investigator, but was at the University of Arkansas at the time he received his EPiQS award. In August 2017, an EPiQS Community-Building Grant was awarded to these three researchers at Rutgers to create a new facility that produces "active substrates," an important class of materials used by quantum materials researchers in a range of investigations. Researchers will receive support to travel to Rutgers, learn how to use the equipment in this facility, and synthesize new substrates to meet their research needs.

The faculty at Rutgers are also pursuing a more formal relationship with EPiQS grantees at nearby Princeton University. Princeton also has a strong investment in materials synthesis, as host of two of the most prominent synthesists (Profs. Cava and Pfeiffer) and a number of Experimental Investigators. The growth of this New Jersey cluster is not accidental—a number of Rutgers and Princeton faculty are alumni of the Bell Labs complex, and hope to bring that same spirit of excellence and collaboration to their future work in quantum materials.

Change for EPiQS emphasizes the importance of facilitating collaboration among awardees, our study suggests that collaborations and interactions among postdocs and graduate students are an important intermediate step that also motivates certain collaborations. Efforts to promote more intra-institutional collaboration, especially those that span the strategies supporting theory, experimentation, and synthesis, should examine opportunities to leverage the informal networks of these very early-career scholars.

# 5.3 Effects of EPiQS on Postdoctoral Researchers through Theory Center and Other Awards

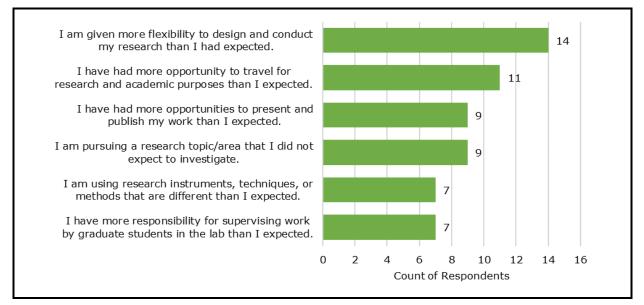
For the most part, the Theory Center PIs stated that the Moore Postdoctoral Scholars enhanced significantly the work being done at those Centers, and contributed to efforts that focused quantum theory on issues relevant to quantum materials. At those Centers, the PIs by tradition keep in close contact with postdoctoral researchers and provide them with active mentoring. At most universities with a quantum materials theory group, the number of faculty in that area is rather low. Adding two or three postdoctoral scholars may end up doubling the number of researchers focused in this area. Several PIs also emphasized that the postdoctoral scholars end up educating the faculty, because they are more familiar with some of the new computational techniques for theory and modeling that are increasingly common in this field.

The Theory Center PIs also claimed that they are much more proactive in seeking out candidates with interesting backgrounds and diverse intellectual traditions. At those institutions, the Moore Postdoctoral Scholars have played a key role in moving the Theory Center PIs to examine new questions and explore new constructs and frameworks, as well as promoting more collaboration between theoretical and empirical work. This enhances the capacity of Theory Center faculty to incorporate of new ideas and new techniques, such as modeling and simulation, in their own work.

The Postdoctoral Scholars in the Theory of Quantum Materials also benefited greatly from their awards and their experiences working in the Theory Centers. Because the Theory Center PIs have tremendous discretion in hiring each set of scholars, the current and former scholars have an eclectic range of backgrounds. At some Theory Centers, scholars were hired out of fields other than quantum materials, such as high energy physics and astrophysics, because the faculty members thought that they could bring a new set of tools and perspectives to the field. The scholars themselves reported that they have been highly engaged and motivated to delve into completely new areas of quantum theory. Some of these scholars were also instrumental in engaging faculty from theory and experimentation in new collaborations, as noted in the previous section.

Postdocs, including those hired through awards other than the Theory Center grants, reported a very high level of satisfaction with their research experiences, as reflected in the survey responses in **Figure 5-3**. They are being trained to use state-of-the-art instruments and equipment and also are being exposed to new research ideas. An important benefit for many postdocs, including the Theory Center scholars, is the opportunity to participate in the EPiQS Postdoctoral Symposium. At this meeting, postdocs supported by EPiQS present their research to each other without any PIs or faculty present. Participants in the 2017 Symposium reported that without the pressure of presenting to senior researchers, they felt more comfortable in advancing their own ideas and engaging in debates over research

approaches and results. Those experiences are an important component in developing postdoctoral researchers into fully-independent research leaders.



## Figure 5-3. Postdoc Views of their EPiQS-Funded Postdoctoral Experiences

In the postdoc survey, a substantial but not overwhelming number of respondents reported that their experiences in their EPiQS-funded positions exceeded their expectations for the quality of research experience gained. When interviewed, postdocs connected these aspects of their research experiences to better prospects for gaining a prominent research position in their next job. Some of the postdocs who felt that their experience did not exceed expectations reported that they already had high expectations before starting, due to the prestige associated with the Moore Foundation. This helps to enhance the overall intellectual environment at these institutions, and also enhances the prominence and prestige of fellowships hosted by these universities.

Postdoctoral researchers interviewed for the study agreed that quantum materials is a legitimate subfield of condensed matter physics, that it is probably the most exciting research area within physics today, and that it is a very promising area for future careers. Virtually all postdocs stated that they plan to stay in this field as they launch their academic careers, and they expect the field to grow in scale and influence in the coming years.

# 6. EPiQS AND U.S. RESEARCH INFRASTRUCTURE IN QUANTUM MATERIALS

In quantum materials, progress is affected greatly by the availability of high-quality samples of synthesized materials. Sourcing materials from researchers in other countries is a regular occurrence, but it introduces many risks: the shipment might be delayed in customs, the package could be mishandled such that the sample suffers from some defect, or the sample may not arrive at all. EPiQS has an explicit goal of making access to both sample materials and advanced instrumentation more convenient and frequent for U.S. researchers in quantum materials.

## Key Findings

- EPiQS funding has supported work by synthesists such that it is easier and more common for U.S. researchers to source sample materials from other U.S. institutions, rather than relying on non-U.S. synthesis researchers.
- EPiQS grantees other than Equipment Development awardees are investing in new laboratory equipment and instruments, providing important infrastructure for future research efforts.

# 6.1 Enhancing U.S. Capacity in Materials Synthesis

Both interview results and the surveys confirmed that (a) the availability of material samples was a problem for U.S. empirical researchers in quantum materials, (b) the capacity to synthesize materials in the United States had declined significantly with the end of the era of large central industrial laboratories, and (c) investments in synthesis and synthesis capabilities were much more favorable in other countries. (Interview subjects commonly referred to China, Japan, South Korea, and Germany as the leading nations in synthesis.) They also agreed that the decision to make materials synthesis a major component of the EPiQS Initiative was a valuable service to the community and addressed a critical need in the U.S. research environment. The Expert Panel supported that assertion, but noted that reviving U.S. leadership in materials would require a long-term investment.

Half of the respondents to the grantee survey indicated that they have had problems acquiring samples for research in the past (see **Figure 6-1**). Of the half who had difficulty acquiring samples in the past, eight of nine acquired at least one material sample from an EPiQS grantee, since receiving their award. Of the other half who had not had problems acquiring material samples in the past, seven of nine (about 78%) had acquired at least one material sample from an EPiQS grantee since the start of the EPiQS initiative. Only two (about 11%) respondents indicated that they had neither experienced a problem acquiring a

material sample for research in the past nor had they acquired any material sample from an EPiQS grantee since receiving their awards.

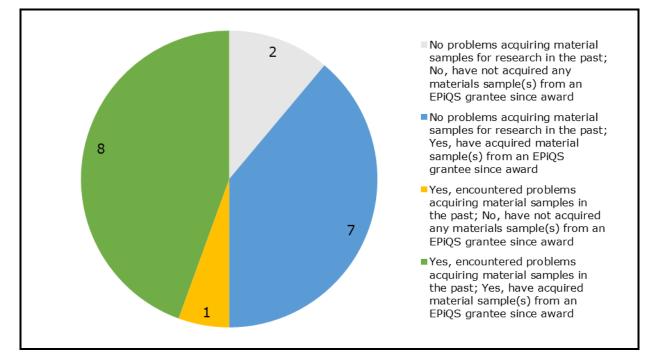
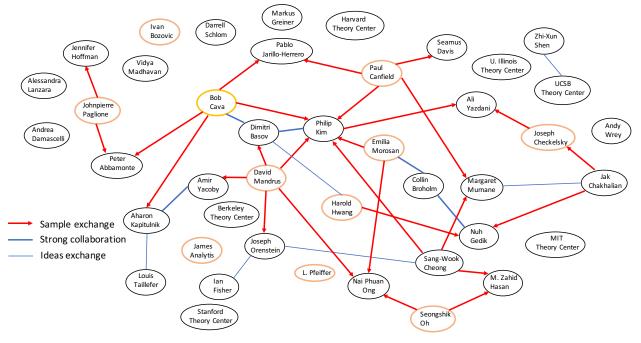


Figure 6-1. Grantees' Experiences in Acquiring Sample Materials

A notable trend that appeared through interviews is the melding of researchers focused on experimentation and those focused on synthesis. EPiQS grantees working in characterization are increasingly aware that the details of synthesis and crystal growth have significant implications for their research. At institutions that house researchers in synthesis, more experimental grantees (and especially their postdocs) are being cross-trained in synthesis, in part so that they can grow some of their own samples. At the same time, some of the younger scholars working on synthesis are reaching out to experimentalists to learn more about techniques in measurement and characterization to advance their own work. While empirical work and synthesis remain distinct competencies, these two legs of the stool may be moving closer together.

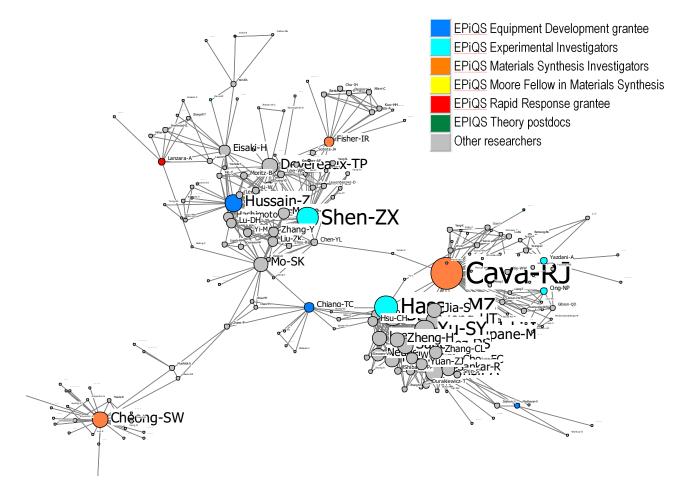
Grantees do report that, thanks to EPiQS, they are sourcing more of their research materials from U.S. synthesis experts—primarily other EPiQS grantees. The Investigator Symposium was frequently referenced as a venue where experimentalists heard about new materials samples from the synthesis investigators and where they first made arrangements to acquire materials. For those experimentalists, access to samples has improved in the relatively short period since the launch of EPiQS. **Figure 6-2**, provided by the EPiQS Program Staff based on information extracted from annual grantee reports, illustrates the extent of collaborations between grantees that grew from interactions at the annual Investigator Symposium. Note that transfers of samples from synthesists are the dominant mode of collaboration in these instances. Awardees who are either Materials Synthesis Investigators or Moore Fellows in Materials Synthesis are highlighted in orange. In some cases, sample materials are being transferred from Experimental Investigators as well. Note that investigators who are not part of a collaboration on this chart may still have joint research with other awardees, but not collaborations initiated at the Investigator Symposium.





The collaboration networks formed by grantees with non-grantee researchers also illustrate the key role of materials availability in joint research. In **Figure 6-3**, we display data drawn from all scientific journal articles published between 2014 and 2017 where at least one coauthor was an EPiQS grantee (although the articles were not all reports of research funded by EPiQS). Each node is an author on an article, and each line signifies that two researchers collaborated on at least five separate articles during this time period. Colored nodes are EPiQS awardees, and in particular, orange nodes denote Materials Synthesis Investigators. The size of each node is a function of the number of collaborations involving that researcher.

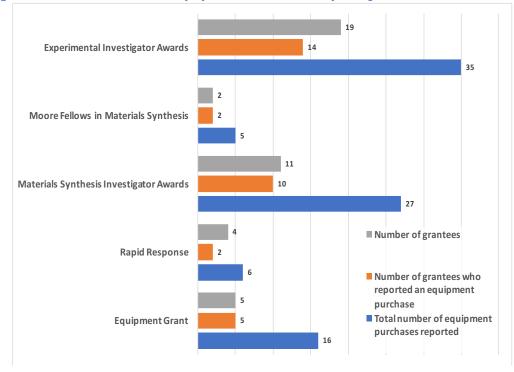
In this figure, we see the particular collaboration patterns of the synthesis researchers. Profs. Robert Cava and Sang-Wook Cheong are prominent collaborators. They show a high degree of "network centrality," meaning that that are central figures in a cluster of collaborations. Profs. Hasan, Hussain, and Shen are also active in many collaborations, but participate in clusters where other researchers are also very central figures. Another key feature of the EPiQS synthesists is that they function as "bridges" between different clusters. Profs. Cava, Cheong, and Fisher all have relationships that reach beyond their respective clusters and involve researchers from a different cluster, or outside of a particular cluster. In network analysis, these individuals are "boundary-spanning" actors— they form relationships that span groups of researchers that normally would not collaborate. These researchers are critical community members, as they help to maintain cohesion between disparate subcommunities and they involve less active community members in their partnerships. Note that Profs. Hasan and Chiang (co-PI on an Equipment Development award to Prof. Madhavan at the University of Illinois) also tend to fill boundary-spanning roles. Identifying grantees who act as connectors illustrates how EPiQS grantees can influence the broader quantum materials research community. Tracking co-authorship relationships in this way also can show how influential these grantees have become, both among collaborators and across different subcommunities.



#### Figure 6-3. Detail of Co-authorship Networks for Selected EPiQS Grantees, 2014 to 2017

# **6.2 Expanding Capacity and Infrastructure through Equipment and Instrumentation**

In Section 4, we noted that almost all EPiQS grantees reported that they purchased equipment or instrumentation with EPiQS funds. To confirm this, **Figure 6-4** is drawn from grantees' annual reports and financial reports between 2014 and 2017. Consistent with the survey responses, most Experimental Investigator and virtually all synthesis researchers (Investigators and Fellows) reported purchasing at least one item of equipment or instrumentation. Grantees reported the cost of the equipment in approximately 65% of instances. Purchases ranged in scale from \$30,000 for a glovebox to over \$1 million for a molecular beam epitaxy system. Not surprisingly, equipment development grantees spent the largest total amount on equipment purchases.





Affirming the survey results, numerous grantees discussed during interviews how they used EPiQS funds to refurbish equipment by replacing old machines with new ones, or to get a particular piece of hardware for a new project. These purchases can provide many important, enduring benefits:

- By modernizing their own laboratory facilities, grantees can perform research on highly-reliable equipment using the most current techniques for quality assurance, measurement, and analysis. This helps to ensure the quality of their findings.
- As one grantee pointed out in an interview, advances in technology and miniaturization now make it affordable to purchase sophisticated equipment and

instruments that were too costly even a few years ago. For example, the cost of a molecular beam epitaxy chamber has declined at a steady pace. EPiQS funds allow grantees to take advantage of capabilities that previously would have required travel to a specialized facility.

- Researchers can elect to allow other faculty at their institutions to use their laboratory equipment for particular experiments. This means that these equipment purchases benefit research performed by non-grantee researchers at the same institutions.
- In many cases, the instruments acquired will be used by the researchers for many research investigations funded by multiple sponsors in subsequent years. This helps those other sponsors, as they can support higher-quality research performed by EPiQS grantees. This also increases the likelihood that EPiQS grantees can develop compelling proposals based on capabilities that they may not have had prior to EPiQS.
- Graduate students and postdoctoral researchers in the Investigators' labs also mentioned the value that they received in learning how to use these state-of-the-art systems. That knowledge will be useful to them in future positions, even if they leave academia to pursue careers in industry.

These factors reinforce the importance of allowing EPiQS grantees to purchase equipment with minimal administrative burden. Some of the equipment purchased is too expensive, and possibly too cutting-edge, to be allowable expenses under typical federal funds. In other cases, grantees can leverage equipment and instruments purchased through EPiQS with those purchased with other funding sources. In several cases, grantees' purchases of equipment were partially supported by federal or institutional funds. The U.S. Department of Defense also announced recently that special research equipment awards were given to Profs. Greiner, Kim, and Yacoby, further enhancing their research capabilities.<sup>13</sup>

<sup>&</sup>lt;sup>13</sup> Department of Defense Announces FY18 Research Equipment Awards. Press Release from the U.S. Department of Defense, April 3, 2018, retrieved at <u>https://www.defense.gov/News/News-</u> <u>Releases/News-Release-View/Article/1483307/department-of-defense-announces-fy18-research-equipment-awards/</u>

# 7. BROADER IMPACTS: THE EPIQS INITIATIVE AND THE FUTURE OF QUANTUM MATERIALS RESEARCH

Given its vision to influence the trajectory of scientific progress on quantum materials, the EPiQS Initiative must reach beyond its pool of grantees and affect the global research community. Catalyzing transformative change requires that the EPiQS Initiative influence (a) the discovery or development of a *potentially transformative* research result and (b) the *realization* of transformative change through a shift at the level of the research community. Eventually (often years later), this change may lead to the *recognition* of that transformative change, for example, through an award by the Nobel Committee.

## Key Findings

- EPiQS played a key role in establishing quantum materials as a distinct field of research in the U.S. and internationally, and that has sparked interest in the field.
- Although there is no evidence that EPiQS influenced other research sponsors to increase funding for quantum materials research, EPiQS helped to focus sponsors' interest in this topic, and those sponsors are providing follow-on funds to support EPiQS grantees' research.
- Evidence that EPiQS is "catalyzing transformative change" in quantum materials
  research can be seen in how topics pioneered by grantees are becoming the focus of
  other researchers in the field.

## 7.1 EPiQS and the Evolution of the Science of Quantum Materials

Interviewees point out that the EPiQS Initiative did not coin the term "quantum materials," but do credit EPiQS with raising awareness and increasing usage of the term and increasing the stature of quantum materials within the research community (see **Figure 7-1**).<sup>14</sup> Interviewees did not provide a single, authoritative definition of the term "quantum materials," but indicate that their peers show a rough consensus on what topics are associated with that label. As stakeholders pointed out, this makes it easier for the field to attract new researchers and also to focus funding by other sponsors. For example, the term "quantum materials" was used in a "basic research needs" report mapping out future directions in DOE support in this area.<sup>15</sup>

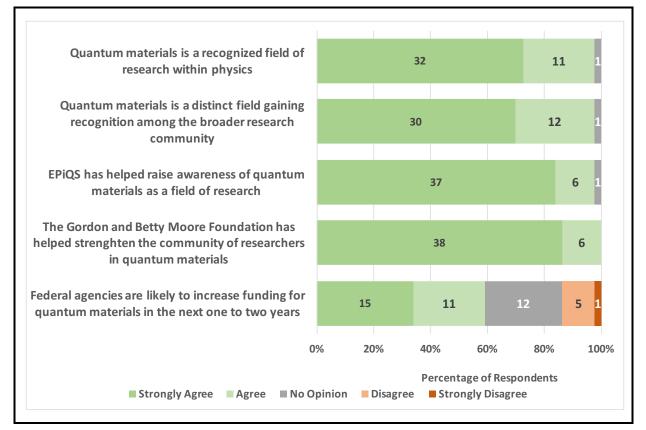
<sup>&</sup>lt;sup>14</sup> Interviewees commonly attribute the coining of the term to a group at the Canadian Institute for Advanced Research around 2007 or 2008.

<sup>&</sup>lt;sup>15</sup> U.S. Department of Energy, Office of Basic Energy Sciences. (2017). *Basic research needs workshop* on quantum materials for energy relevant technology. Washington, DC.

Interviewees offered various examples where activities supported and catalyzed by EPiQS funding brought the field of quantum materials to a new level of prominence in the scientific community:

- By convening special seminars or events at major scientific conferences, EPiQS has helped expose more of the physics community to the science of quantum materials. Stakeholders interviewed (including grantees, postdocs, and federal program managers) report seeing a greater number of special panels and talks on quantum materials at major conferences in physics.
- Review articles and similar publications by EPiQS grantees in major journals also show that journal editors accept this term as a meaningful identifier. The recent special issue in *Nature* on quantum materials, involving several grantees and with support from EPiQS and the Simons Foundation, can be used as evidence that quantum materials has "arrived," as one researcher put it.
- A few interviewees highlighted the role that the new journal *npj Quantum Materials* (*NQM*) has played in bringing together articles in this field in one venue. Previously, articles on quantum materials research appeared only intermittently in journals such as *Physics Review Letters*, *Nature Physics*, and *Nature Materials*. Having a journal where these articles appear together has raised visibility substantially. These interviewees also observed that *NQM* has risen in influence faster than almost any other scientific journal, further solidifying the position of this field.

## Figure 7-1. EPiQS Grantee Assessment of Quantum Materials Research



As one immediate measure of the impact of EPiQS on the field of quantum materials, awardees have already published a substantial number of articles contributing to the literature in this domain. A search of the Web of Science database of journal articles found 487 articles published between 2014 and 2017 that cited funding from EPiQS in the acknowledgements (see Error! Reference source not found.). Of those, 150 appeared in the journal *Physical Review B*, followed by *Physical Review Letters* with 71. **Table 7-1** Table 7-1:

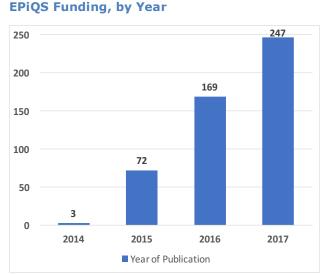


Figure 7-2: Publications of Articles Citing

Publications with EPiQS Funding in High-Impact Journals, 2014-2017below shows the number of articles that appeared in the most widely-cited journals (those with an impact factor of 5 or above).

### Table 7-1: Publications with EPiQS Funding in High-Impact Journals, 2014-2017

Publication Title	Articles
Nature Materials	7
Nature	9
Science	19
Nature Physics	19
Physical Review X	14
Nature Communications	27
Nano Letters	22
Proceedings of the National Academy Of Sciences	14

It is important to note that EPiQS grantees, as high-achieving researchers, were already prolific authors of research articles prior to their awards from the EPiQS program. **Table 7-2** shows the total number of articles authored by grantees in each funding strategy by year, starting in 2012, and then the number of their articles that acknowledge EPiQS funding through 2017. Across all of these groups, the share of their published articles supported by EPiQS has increased, from 12% in 2015 to 43% in 2017. Within each group, the share has also increased each year (except for the Moore Fellows in Materials Synthesis, due to the small number of grantees and publications). Most groups produced fewer articles per researcher in 2017 than 2016, but as mentioned in **Section 4**, a number of grantees

stated that they reduced their number of articles authored each year to spend more time on ensuring that their research produces higher-quality outputs.

Group	2012	2013	2014	2015	2016	2017
EPiQS Equipment Development grantees	69	84	74	84	75	65
EPiQS funded				1	2	3
EPiQS Experimental Investigators	161	150	159	171	160	157
EPiQS funded				27	63	66
EPiQS Materials Synthesis Investigators	195	193	174	230	230	201
EPiQS funded			2	32	66	83
EPiQS Moore Fellows in Materials Synthesis	12	5	8	5	6	8
EPiQS funded					5	5
EPiQS Rapid Response grantees	53	32	46	39	54	35
EPiQS funded				3	5	11
Moore Postdoctoral Scholars (theory)	34	42	64	56	73	103
EPiQS funded				10	35	74

Table 7-2: Articles Published Per Year by EPiQS Awardees in Different Funding Strategies,2012 to 2017

It is more difficult to determine how many of these articles report significant advances in the science of quantum materials, and to what extent EPiQS was responsible for enabling such advances. The international expert panel reported on what the members considered to be the most important achievements in various topic areas in quantum materials, and the achievements by EPiQS awardees. The most significant number of contributions was in studies on the topological effects of solids. The panel cited in particular work by Profs. Oh, Hasan, Analytis, Ong, Cava, Moore, Orenstein, Fu and Hughes as contributors of key developments in theory and experimental results. The panel notes that interest in this area was sparked by observations by Prof. Hasan and colleagues of 3-dimensional topological insulators, but that the work of EPiQS grantees has extended into topics such as Weyl semimetals, and early indications of the potential identification of topological superconductors came from work by Prof. Yazdani.

Other key advances were noted in the study of 2D materials, studies of spin liquids and complex magnets, new measurement techniques, and the development of new theoretical concepts. The panel pointed out the large body of work emanating from the Theory Centers, particularly work on the understanding of strange metals pioneered by Profs. Balents and Sachdev, and the application of holography to explain unusual quantum properties. Key measurement capabilities advanced through EPiQS funding can be seen in scanning tunnel spectroscopy, microwave impedance imaging, scanning optical microscopy, and techniques in angle-resolved photoemission spectroscopy.

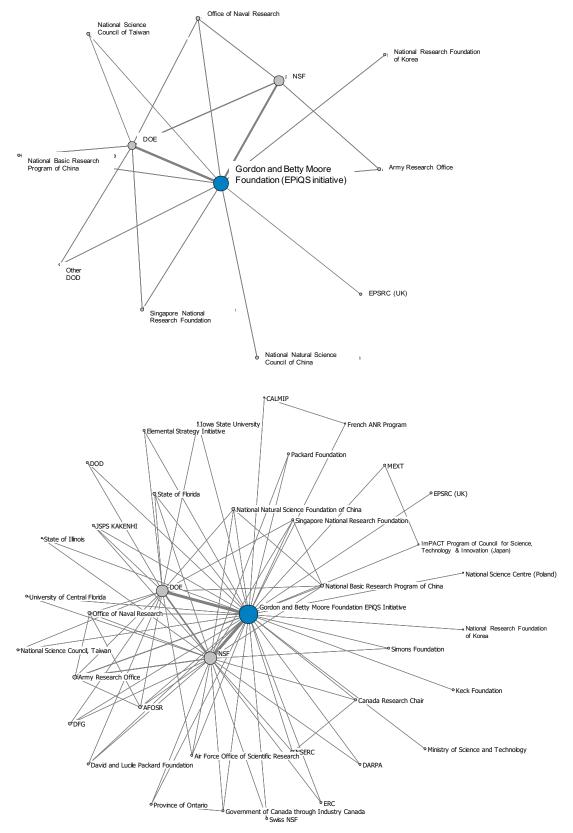
## 7.2 Influence of EPiQS on Other Research Sponsors

As noted in earlier sections, quantum materials was a topic of growing interest in the scientific community prior to EPiQS, and this is reflected in the behavior of research sponsors. Looking retrospectively at scientific journal articles that could be classified as work on topics in quantum materials, U.S. federal agencies are cited as funding sources for a growing number of articles. The dominant funders are the DOE and NSF, with each supporting about 200 quantum materials articles published in 2008, rising to approximately 1100 articles funded by each agency in 2017. (Note that in some cases, both agencies contributed funding to the same article.) The 247 articles published in 2017 with support from EPiQS makes the Gordon and Betty Moore Foundation the fourth most active funder of U.S. research articles in this field, somewhat behind the National Natural Science Foundation of China.

Although there is no indication of the growth in actual federal funding levels for quantum materials research, it is unlikely that EPiQS is crowding out existing investments. In fact, the initiative's emphasis on "people" and innovative research plans, in addition the flexibility in how grantees use EPiQS funding and its substantial support to materials synthesis, makes EPiQS funding complementary to federal programs rather than duplicative. Federal program managers believe that EPiQS is providing support for areas of research that are not viewed as appropriate for federal support—in particular, in its support for developing new experimental techniques and supporting "high-risk" research. One program manager commented that most of his research funding goes towards incremental research that provides a foundation for the field—what he termed research that "keeps the lights on." The breakthrough research supported by EPiQS relies in large part on that growing base of incremental knowledge. At the same time, another program manager stated that his program does try to support more "cutting-edge" and ground-breaking research when it can. He tracks how many articles acknowledge funding from both his program and from EPiQS, and views that data as evidence that his PIs use his funding for potentially transformative work.

**Figure 7-3** illustrates the role of EPiQS in the funding environment. The top figure depicts the foundation's co-funding relationships for journal articles on quantum materials published from 2014 to 2015, and the bottom figure is the same data for 2016 and 2017. In this chart, a link between two organizations denotes that an article acknowledged funding from both sources simultaneously. The size of the sponsor's bubble is a measure of the number of co-funding relationships for that organization—in technical terms, sponsors with larger bubbles are more central to the overall network. Note that between the two time periods, the Gordon and Betty Moore Foundation has established itself as a prominent partner not only to NSF and DOE, but to Department of Defense agencies and some non-U.S. funders as well. This evidence of co-funding in research topics illustrates how EPiQS can leverage its resources through coordination with federal agencies.





EPiQS grantees report that since their awards, they have received funding from federal sources based on their EPiQS-funded research. DOE grant records show, for example, awards to Profs. Analytis, Mahavan, and Ong for newly-initiated projects related to topological materials. Prof. Analytis also received a \$300,000 grant from the NSF in 2016 to study the nature of Weyl semimetals. The EPiQS expert panel review notes that Prof. Analytis made an important contribution to this topic in 2015 through his EPiQS work, studying Weyl semimetals in crystals. Several other grantees received new NSF grants related to their work. The expert panel also discusses how the work of Profs. Kapitunik and Yacoby on transport measurements in quantum materials has attracted new support from federal agencies. This offers evidence that at a minimum, federal agencies feel that EPiQS grantees are working in areas promising enough to commit their own funding as well.

# 7.3 Specifying "Transformative Change" in the Field of Quantum Materials

Various stakeholders discussed how the EPiQS Initiative could catalyze broad, transformative change in the field of quantum materials. One interviewee put the situation aptly: "[EPiQS grantees] should not just be following the herd. They shouldn't even be leading the herd. They should be out in front, showing the leaders of the herd where to go." Another interviewee stated that researchers "vote with their feet," so observing whether the community starts to shift its attention to a particular new material or new concept is the best indicator of transformation.

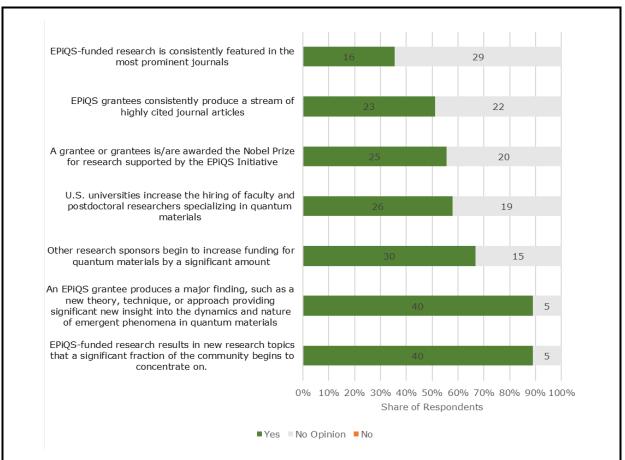
This list below appears in the 2015 Strategic Review of EPiQS as possible examples of potentially-transformative research developments.<sup>16</sup>

- Quantum materials of far better quality (impurity control, crystal size, film quality, etc.) than previously possible
- Synthesis of new members of known classes of quantum materials
- Discoveries (synthesis) of entirely new classes of quantum materials
- Development of new synthesis methods for quantum materials
- Discoveries of new types of emergent electronic behavior
- Theoretical explanations of known emergent electronic behaviors
- Theoretical predictions of new types of emergent phenomena

<sup>&</sup>lt;sup>16</sup> Gordon and Betty Moore Foundation. 2015. Final EPiQS Strategy Review Appendix I – Updated Initiative. Palo Alto, CA: Gordon and Betty Moore Foundation, p. 5.

 Significant improvement of existing and development of new experimental techniques, which enable scientists to collect information about quantum materials that was previously inaccessible

**Figure 7-4** below shows the judgments expressed by grantees in their survey responses to the question regarding tangible examples of "transformational change." The answers showing the highest consensus are similar to the above list: the disclosure of a major new finding or development, and a resulting shift in the attention of the research community as a whole based on that discovery.



## Figure 7-4. Views of Hypothetical Initiative Outcomes that Constitute "Transformative Change"

Despite the fact that the impact of many ground-breaking discoveries in the past took years to unfold, there are instances where EPiQS-funded research has produced results that garnered very immediate and intense attention in the research community. The expert panel noted in the area of 2-dimensional materials, early discoveries by grantees including Profs. Jarillo-Herrera, Kim, and Heinz are "opening several new research directions" that are the focus of work by younger generations of scientists. Another key aspect of the work enabled by EPiQS is its support for new tools, from conceptual frameworks to measurement instruments, that are now adopted by other researchers. The expert panel notes that the Theory Centers pioneered the new holographic approach to analyze strongly correlated metals. Recent work to develop a new approach in scanning tunnel microscopy, by Profs. Davis, Schlom, and Shen, is cited as a method that enables a new class of experiments examining key classes of metal-oxide compounds. Going forward, the EPiQS initiative might benefit from methods that connect the topics emerging in the quantum materials literature to enabling methods and approaches developed by EPiQS grantees. Beyond simple citation counts, this could involve a study of the nature of citations to grantees' articles, putting (for example) more weight on citations that appear in the theory or methods sections of later articles. This can be direct evidence that the community is adopting the thinking pioneered by EPiQS researchers, as an early indicator of potential transformation.

# 8. IMPLICATIONS FOR FUTURE SUPPORT OF QUANTUM MATERIALS RESEARCH

The record of activities and accomplishments of the EPiQS initiative to date provides initial data to inform decisions about future efforts to ensure that the initiative has lasting and substantial impact. We examine three issues that may influence those decisions.

**Continuation of support for quantum materials research.** The decision by the Gordon and Betty Moore Foundation to launch EPiQS made a substantial impression on the research community, and the interest in EPiQS and its results has only grown. Although EPiQS funding awards will expire in 2018 and 2019, the initiative only recently gained broad recognition in the scientific community, and the research results are just now entering the literature. Discussions with a wide range of stakeholders, including researchers not funded by EPiQS and federal program managers, reflect a consensus that the foundation should be aware of the implications of ending EPiQS without any follow-on initiative. The broader community would see this decision as a signal that EPiQS did not produce the desired results, and that perhaps the field of quantum materials is not a worthwhile area of focus. Several stakeholders noted that in fundamental research fields, time is the most important factor in achieving substantial change in the structure and behavior of research communities. The time horizons for discoveries tend to be fairly long, and traditional disciplinary cultures and norms are not easily altered. These individuals felt that at least another five to ten years of concentrated support and effort by EPiQS would be needed to ensure that its impact was sustainable.

**Changing the reach and scope of EPiQS.** The relatively mild criticisms of the design of the EPiQS program focused on two aspects. First, by funding a relatively small number of investigators, EPiQS could be seen as too exclusive. Observers agreed that while EPiQS funded top U.S. researchers in quantum materials, it did not fund ALL such researchers. This leads to rampant speculation as to why certain researchers were not funded, or what factors other than merit were involved in the selection of awardee. This kind of speculation is inevitable, even if it is baseless. As a response, the EPiQS initiative could broaden in two ways: funding more top researchers who are recognized leaders in the field, or funding some lesser-known researchers who have very promising ideas and exhibit creative approaches—what one grantee called "diamonds in the rough."

Both options carry risks. First, expanding the number of grantees is possible to a point, but a clear strength of EPiQS is that it has a fairly tight-knit community. As one grantee put it, the size is just right so that during the Investigator Symposium, an individual can meet and talk to just the right number of peers. In most other meetings, there are too many people and insufficient time to have such discussions, which have proven important for launching new collaborative research efforts. More analysis may be needed to identify the "tipping point" where the size of the grantee cohort becomes unwieldy for facilitating strong collaborations.

Second, attempting to find "hidden gems" in the research community will, in part, mean relaxing the use of the "people-centered" approach to awardee selection. An award may still target an individual with significant potential, but a less-prominent researcher will almost certainly have a less comprehensive record of achievements than the current cohort of grantees. This makes it more difficult to evaluate that researcher's capabilities in carrying out an ambitious program of research, or in judging the most promising opportunities to pursue.

One variation to address these two issues is to have a larger number of targeted activities that encompass non-grantees. For example, the Investigator Symposium could be expanded to have a limited portion where a larger pool of invited guests is present. Another possibility is to provide specific subawards that provide targeted, formal support efforts where an EPiQS grantee has chosen to work with a more junior non-grantee colleague. These types of measures are designed to extend the reach of EPiQS beyond its pool of grantees, but with a modest additional investment.

Identifying and tracing longer-term impacts. Our study identifies a few areas where the funding from EPiQS can have impacts far beyond its funding period. One important area is its impact on postdocs, especially those outside of the Theory Centers. The EPiQS staff may be able to devise a method to track more closely where those postdocs (including Theory Center postdocs and those supported through other awards) go once they have left their EPiQS-funded positions, and what work they pursue related to research of EPiQS grantees. In the context of the number of postdocs at U.S. institutions focused on quantum materials, the number of positions supported each year by EPiQS is substantial. The National Science Foundation's survey of graduate students and postdoctoral researchers shows that in 2016, nonfederal domestic sponsors (including foundations like the Moore Foundation) funded a total of 337 postdoc positions in physics at U.S. universities. That number covers all areas of physics, including but beyond quantum materials. Between the Theory Centers and Investigator Awards, EPiQS is supporting perhaps 50 to 60 of those positions. While a relatively small share of all U.S. postdocs in physics (estimated at 2,819 in 2016), this is a large enough group that that they could have an important cumulative effect on expanding the pipeline of young researchers launching new careers in quantum materials.

We also point out the tremendous benefits gained by allowing grantees to purchase new equipment. This is another aspect of the program that is relatively easy to track (based on grantee reports) and contributes directly to future research results. Similarly, tracking research collaborations involving grantees (both through self-reporting and co-authorship data) can provide verifiable evidence of broader community-level impacts of EPiQS funding.

In summary, we find that the EPiQS initiative was designed with great care and an appropriate scale and approach, and was implemented in a way that clearly maximized its chances of achieving the desired change in the field of quantum materials. Our analysis shows early signals that EPiQS will at some point support the type of research that leads to transformative discoveries, although the time horizon for payoff is uncertain. By continuing to leverage funding from federal sources, and by focusing its grantees on ambitious, exciting, and long-term research problems, EPiQS is making a valuable contribution to the field that is not replicated by any other funding program.

# 9. GLOSSARY OF ABBREVIATIONS

AFOSR	Air Force Office of Scientific Research
CAS	Chinese Academy of Sciences
CIFAR	Canadian Institute for Advanced Research
CNPq	National Council for Scientific and Technological Development (Brazil)
DARPA	Defense Advanced Research Projects Agency
DFG	German Research Foundation (Deutsche Forschungsgemeinschaft)
DOD	Department of Defense
DOE	Department of Energy
EPiQS	Emergent Phenomena in Quantum Systems
ERC	European Research Council
MEXT	Ministry of Education, Culture, Sports, Science and Technology (Japan)
MOST of China	Ministry of Science and Technology (China)
NQM	npj Quantum Materials
NSERC	Natural Sciences and Engineering Research Council
NSF	National Science Foundation
PI	Principal investigator