

## Message from the Newsletter Editor



Taylor Juran

Dear FECS Members,

We are excited to share our Spring 2021 newsletter with you! We hope this letter helps the physics community feel a bit more connected, as the global epidemic has caused a sense of disconnection for many of us.

In this edition, we share information regarding our activities at the March and April meetings, insight from APS, and an overview of the survey that FECS members recently did concerning their desires for the forum as well as their thoughts on how COVID has affected their job prospects and work.

We also feature a special topic article from one of our members, we hope to continue to include these interesting pieces and invite you to get in touch with us if you are interested in contributing a piece for FECS content.

I would like to sincerely thank all of the contributors to this issue of the FECS newsletter, for their hard work and insight. Of course, I would like to thank all of our readers and FECS members as well.

Suggestions, comments about the newsletter, and article contributions are always very welcome, and you can reach me with these at our Facebook “APS Forum for Early Career Scientists - FECS” (<https://www.facebook.com/APSFECS>).

You can also reach me and other FECS members on APS Engage (<https://engage.aps.org/fecs/home>). I hope to connect with you in the future!

Sincerely,

Taylor Juran  
Communications Officer

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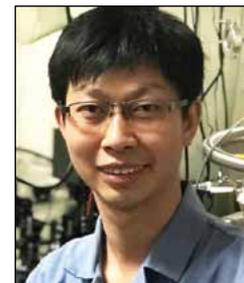
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*Views and opinions expressed in articles are those of the author and are not necessarily shared by the editor or the APS/FECS.*

*Taylor obtained her Ph.D. from Binghamton University, State University of New York. After completing her Ph.D. she joined Materials Design Inc. as a Support and Applications scientist. She is interested in computational modeling of battery materials for sustainable energy.*

# Message from the Chair

Shaowei Li, Chair



Shaowei Li

Dear FECS Members,

Welcome to the 2021 FECS newsletter! The past year has been unusual for everyone, including FECS. In light of the pandemic, a lot of academic events have been canceled, and many others are converted to virtual. FECS turns five years old during this special time. Established in 2016, the objective of FECS is to enhance APS's ability to meet the needs of early-career scientists, to offer them support services, and to provide them with an opportunity for increased inclusion and participation in the activities and decision-making of the physics community. We continue working towards these goals during the global COVID pandemic. Here I would like to present you with a summary of what we have done in the past few months.

In February 2021, FECS participated in the APS virtual congressional visit day to discuss the topics that concern the interests of young scientists with house representatives. During this visit, we brought up the issue of the impacts of COVID on young scientists and requested robust funding increases in the COVID relief RISE act for the DOE Office of Science, the DOD Basic Research Organizations, NIST's Scientific and Technical Research Services (STRS), and the NSF. We are glad to see that this request received bipartisan support. The RISE Act is providing \$25 billion to independent research institutions, public laboratories, and universities throughout the country to continue their work on thousands of federally backed projects. During this visit, we also bring up other important issues such as the Helium crisis, methane as a greenhouse gas, sexual harassment in academia, etc.

You may have also heard several times from us about the "Supporting Early-Career Researchers Act", which we are working together with APS leadership to push for. This act authorizes NSF to create a fellowship program that will enable recent Ph.D. graduates and postdocs to conduct independent research for two years. We aim to set up a program similar to NIH K99, Roland fellowship at Harvard, Miller fellowship at Berkeley to allow early-career scientists to become more competitive job candidates – in academia, the national labs, or the private sector – and even stronger contributors to our nation's research enterprise. Meanwhile, this fellowship aims to improve diversity in academia. Studies have shown that a large portion of URM students decide not to stay in academia at the stage of postdoc. We hope this NSF-funded fellowship program can help reduce stereotypes in academia and provide additional support

to the URM groups. I am happy to share with you that this act has passed the House and was introduced to the Senate on May 18.

This year, APS held its first virtual March and April meetings. Even though we did not meet in person, FECS worked with other APS units to make these meetings as successful as before. This year, FECS held three March meeting sessions. In "Young Investigators in low dimensional quantum materials", we invited many outstanding young players in low dimensional materials to share their exciting results. In "What Do Early-Career Physicists Do? A Diversity of Career Options" (co-host with FIAP), we invited several young physicists in different industries including finance, data science, quantum information science, and software engineering to provide their first-hand experience on how education in physics helps during their daily work. In "Top Quality Early Career Science in Europe (co-host with FIP)", we invited several top-tier young researchers in Europe to share their latest results. We are glad to see that all these sessions are well-attended. Indeed, the "What Do Early-Career Physicists

*Shaowei Li is a Heising-Simons Postdoctoral Fellow in the Physics Department, University of California Berkeley. His research focuses on developing a novel imaging technique combining laser and a scanning tunneling microscope (STM) to shatter the diffraction limit and probe the inhomogeneous properties in low dimensional materials. The desire for observing finer details using optical microscopy particularly in bio-science and material-science is pushing technology developments beyond the diffraction limit. The coupling of photon excitation with electron tunneling at the junction of a scanning tunneling microscope combines the femtosecond sensitivity of a laser and the Angstrom resolution of tunneling electrons. The joint fs-Å resolution will provide a new window for viewing the unique ultrafast dynamics of individual nano-scale objects. Shaowei received his Ph.D. in physics from UC Irvine in 2017. Prior to that, he received his bachelor's degree in physics from Nankai University in 2010. He spent a year as a postdoctoral fellow at Northwestern University before joining UC Berkeley. His past work involves probing the physical and chemical properties of single molecules and low-dimensional materials with optical techniques and STM.*

Do? A Diversity of Career Options” was one of the most populated sessions during the March meeting week.

FECS also held a poster competition during the March meeting. The winner this year is Aminur Rahman from the University of Washington (Poster: Physics-based models and simulations of cancer drug response in solid tumors). The two runner-up winners are Antoine Lainé from SISSA, Italy / LPENS, Université de Paris (Poster: Amplitude Nanofriction Spectroscopy), and Ziyu Ye from the University of Delaware (Poster: Computational Reverse-Engineering Analysis for Scattering Experiments (CREASE) Applied to Self-Assembled Polymer-peptide Conjugate Solutions). Meanwhile, FECS offered mini “travel” grants to cover the cost of registering for the 2021 virtual March and April meetings.

FECS continues to promote diversity and inclusion in the physics community. This year we are setting up a unit award to recognize and celebrate the young individuals that embrace diversity and inclusion across the physics community. If you know someone who has made important contributions to this effort, please keep an eye on our “call for nomination” which will arrive at your mailbox soon.

Finally, we hope everybody is staying safe and doing well during this challenging time. FECS continues working hard to support you!

Best,  
Shaowei Li  
Assistant Professor, University of California, San Diego

## April Meeting Mini Grants

**Kevin Ludwick, Treasurer**

For this year’s April Meeting, FECS offered mini-grants to cover the registration fee for selected applicants. Applicants had to be FECS members, recent PhD recipients (past 5 years), and present a poster or talk at the meeting. Women, underrepresented minorities, and candidates who can clearly demonstrate a need for funding were encouraged to apply. Ten people were selected:

Ewerton Belchior Batista das Chagas,  
University of Campinas (UNICAMP)

Angela Burger, Oklahoma State University

Arjun Chhetri, University of Delhi

Sotirios Karamitsos, University of Pisa

Ali Kheirandish, Pennsylvania State University

Rohit Kumar, Panjab University

M.A. Muktadir, North Carolina A&T State University

Cody Parker, Cyclotron Institute, Texas A&M University

Richard Ruiz, Institute of Nuclear Physics,  
Polish Academy of Sciences

Paul Terman, Wesleyan University

Congratulations to the winners of the mini-grants! We hope you continue to excel as early career scientists and members of FECS!



Kevin Ludwick

*Kevin obtained his Ph.D. from the University of North Carolina at Chapel Hill. After a two-year postdoc at the University of Virginia, he became an assistant professor at LaGrange College in 2015, and he is the Pre-Engineering Dual Degree advisor there. His research is in theoretical cosmology, pertaining to dark energy and dark matter models.*

# A Non-Sci-Fi-ish Take on Machine Learning for Scientific Discoveries

Aashutosh Mistry



Aashutosh Mistry

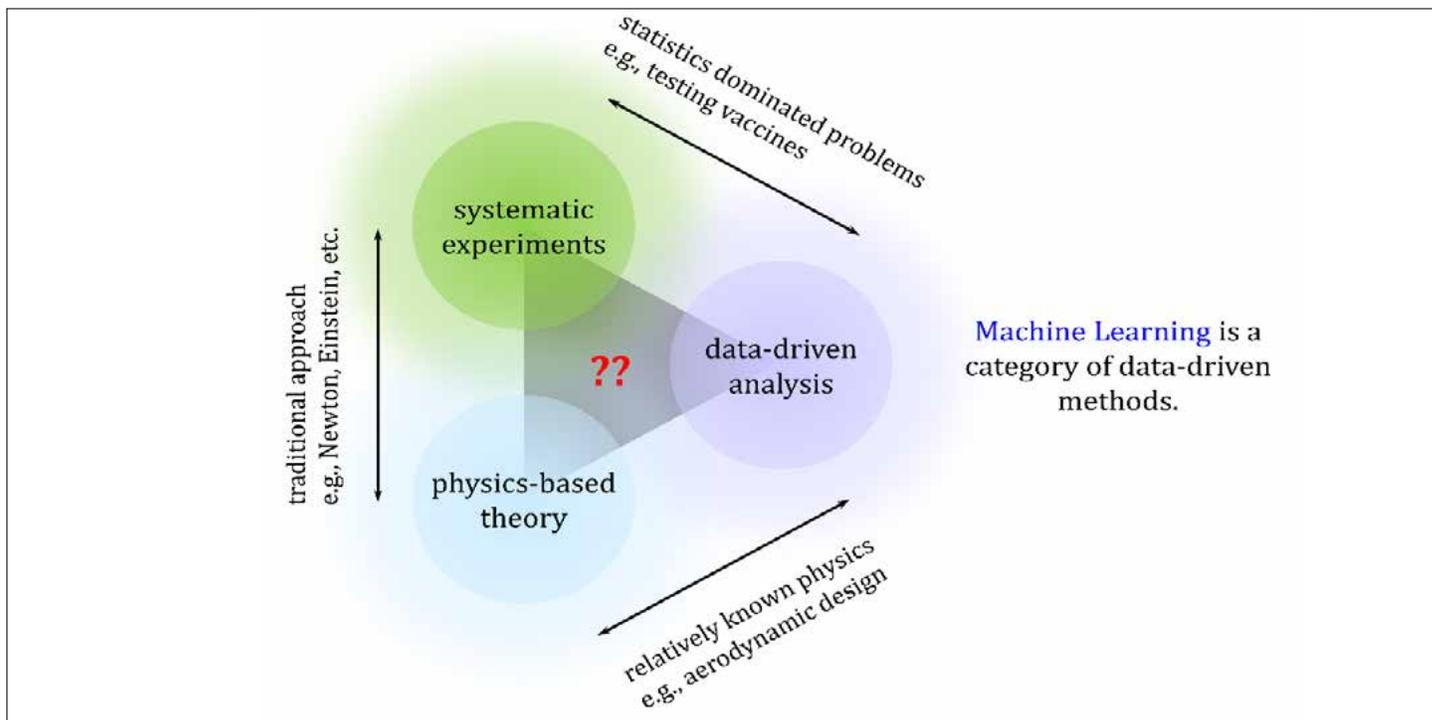
Picture us learning to speak. In our early childhood, we used to rely on what we see and hear to connect words to physical entities, and then utter the same words whenever we wanted to call out the specific entities. For example, we called a dog, a dog just because everyone around us called it a dog. Over time, as we got formally educated in grammar rules, we would express our thoughts and feelings without relying on such explicit correlations. These two learning approaches are fundamentally different. The former one churns the available information to identify common trends to be mimicked. While the latter one uses rules to create prose. Their relative importance is context specific. This analogy extends beyond our linguistic progress and equally describes scientific discoveries (here discoveries are meant in a broader sense, ranging from identifying new physical laws like relativity to inventing new devices such as lithium-ion batteries). In scientific terminology, the first approach is data-driven; while the second is physics-based. Both rely on experiments to study the underlying phenomena and subsequently design or control behavior. Such predictive understanding is central to scientific discoveries. Machine learning – a set of computer algorithms identifying trends from data – generalizes the statistical techniques used to conventionally analyze data. In the following discussion, we will see how machine learning affects our approach to scientific discoveries.

Figure 1 pictorially describes these three pillars – experiments, physics, data – and different investigative paradigms. The traditional approach to discoveries has been either to formulate physical theories to explain experimental observations (e.g., Newton’s law of gravity for why an apple falls downward) or perform measurements to test theories (e.g., Eddington’s 1919 observations of a solar eclipse is one of the proofs for Einstein’s general theory of relativity). This approach is more commonly found in physical sciences. In contrast, biological and social sciences have typically relied on data-driven interpretations of controlled experiments, partly given the multitude of factors that can influence system behavior therein. For example, testing how helpful a particular vaccine is by tracking groups of vaccinated against placebo-treated participants. The physics versus data-based nature of analysis translates to the kinds of insights available following each approach. The data-driven analysis provides *correlations*, while the physics-based formalism elucidates *causations*. The correlations are only valid for the systems that have been explicitly examined; in the

vaccine example, the usefulness of a specific vaccine for someone with different physiology or anatomy cannot be guaranteed beforehand (reading suggestion – *The Formula: How Algorithms Solve All Our Problems ... and Create More* by Luke Dormehl). Alternatively, the causal structure of physics describes a more fundamental reality such as every object on earth experiences an equivalent gravitational pull. Often the choice of one approach over the other is based on the primary objective of the scientific investigation and associated constraints on time, efforts, etc.

As our understanding of material behavior matured and with the advent of computing in the 20th century, an alternate paradigm of high-performance computing has evolved. Herein the physics-based governing equations are solved to generate datasets of material or system behavior for different conditions. Afterward, the data is analyzed to identify materials or systems of interest. Seemingly different but conceptually similar ideas like computer-aided design, high-throughput material screening, etc. fall in this category. A relatable example of this is the design of aircraft shapes. Computational Fluid Dynamics (CFD) is used to simulate airflow around a given shape and in turn, estimate its flight performance. As compared to testing out every shape practically, e.g., in wind tunnel experiments, this is a cheaper alternative.

As computing became more accessible and powerful, it created a space for statistical algorithms processing a vast amount of information (i.e., the machine learning methods). Given the statistical nature, its most visible scientific applications have been wherever large experimental datasets are available, for example, image analysis, global positioning system (GPS) mapping, weather sensors, and self-driving laboratories. The key improvement over the conventional data-driven analysis of experiments is the scale of the datasets and complexities of the underlying correlations. Conversely, when physics is relatively known, machine learning can predict behavior without having to solve for physics every time. In the aircraft design example, machine learning can reasonably predict the effect of minor shape changes to the resultant airflow pattern and flight performance. This further reduces the efforts and allows one to examine more design variations than previously accessible. In both contexts, machine learning essentially creates reduced-order models and provides better predictions or



minimizes efforts. Such reduced-order models natively bridge physics across scales and are helpful to multiscale theories.

The relevance of machine learning in either of these is philosophically clear, while the implementations would evolve over time. Instead, going back to Figure 1, the traditional approach of connecting experiments and physics has been relatively uninfluenced by machine learning. This context is particularly demanding for machine learning since the causality is to be identified from limited experiments, while the present-day machine learning is suited to finding correlations from large datasets (an interesting read – *The Book of Why: The New Science of Cause and Effect* by Judea Pearl & Dana Mackenzie). A possible approach is to cleverly combine physics-based theories with machine learning to interpret experiments. Herein physics will provide the causal structure and decrease data overheads.

All in all, machine learning would change our approach to scientific discoveries in the days to come. For example, our recent article *How Machine Learning Will Revolutionize Electrochemical Sciences* (doi: 10.1021/acseenergylett.1c00194) discusses different emerging applications in electrochemical systems like batteries, CO<sub>2</sub> conversion, etc. It would be curious to see how machine learning helps create a better, cleaner, greener future for everyone.

### Acknowledgments

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Figure 1. Systematic experiments, physics-based theories, and data-driven analysis have been three pillars of scientific progress. Historically, a combination of any two of these has been employed. With the advent of machine learning techniques, we should be able to seamlessly combine the three to minimize efforts and shorten the timeframe for discoveries.

*Aashutosh Mistry obtained his Ph.D. from Purdue University. He is currently a Postdoctoral Appointee at Argonne National Laboratory. Where he examines thermodynamic and off-equilibrium behavior of materials (e.g., transport, reaction). He is curious about leveraging such fundamental insights for designing the next-generation energy storage systems.*

# Brief Insights from the Fall 2020 APS FECS survey

Wennie Wang, Member-at-Large



Wennie Wang

In the Fall of 2020, members of the APS FECS were invited to participate in a survey with the aim to gather recommendations on what FECS should focus on for future meetings and resources and to gauge the impacts of COVID-19 pandemic on members' work experiences. Of the over four thousand members in FECS, we received 170 responses. As an incentive, we gave away \$50 Amazon gift cards to five randomly selected, anonymized participants. Below are brief highlights from the survey.

As of 2020, FECS as a whole is composed predominantly of student members (62%), followed by early-career scientists (25%), regular members (11%), and a handful of senior/all-life members. Approximately 65% of members in FECS identify as male, 21% as female, and 0.2% as non-binary, with 5% not specifying. These demographics are somewhat reflected in the demographics of survey respondents. Figure 1 shows a breakdown of the years since earning a PhD of the survey respondents. Of those who participated in our survey, approximately 55% identified as male, 30% identified as female, and 0.5% identified as non-binary; 12% did not respond.



Figure 1: Breakdown of respondents in 2020 FECS survey for years since earned PhD. Those in the N/A category are either undergraduate or masters students.

When asked what kinds of career resources and training FECS should focus on providing, career development and job search resources were ranked highest, followed by mentoring resources and resources for international researchers. Conference travel stood out as the type of financial support FECS should focus on providing, followed by grants for professional development and travel for short- and medium-term research collaborations. As most respondents indicated interest in an academic career track, academic career sessions were ranked highest as the sorts of sessions recommended for FECS to sponsor. A breakdown of respondents' reported intended career goals is shown in Figure 2.

Finally, we asked about the impact of COVID on our members. More than 65% of respondents have resided in the U.S. during COVID and most reported a high to extreme impact in the local area. Over half agree or strongly agree that they receive adequate information from their institute and that their institution is prioritizing safety in the response planning. Interestingly, when asked whether COVID would significantly affect the ability to continue in the intended career trajectory, the responses were spread relatively evenly between disagree and strongly agree. Nevertheless, over 60% of respondents responded to experiencing a diminished ability to perform work and to communicate with colleagues and/or supervisors/advisers.

As members of the Executive Committee with FECS, we would like to thank all the respondents for their input and time. This survey provided valuable feedback to the FECS Executive Committee on efforts and resources to focus on in the future, particularly in the context of the recent pandemic, and we will keep these and other findings in mind for future efforts.

*Wennie Wang is a computational materials scientist and currently a postdoctoral scholar at the Pritzker Institute for Molecular Engineering at the University of Chicago. She earned her B.S. in Materials Science and Engineering at MIT in 2013 and her PhD in the Materials Department from UC Santa Barbara (UCSB) in 2018. Her research interests include first-principles methods for energy applications and currently encompass the study of complex oxides for water-splitting applications.*

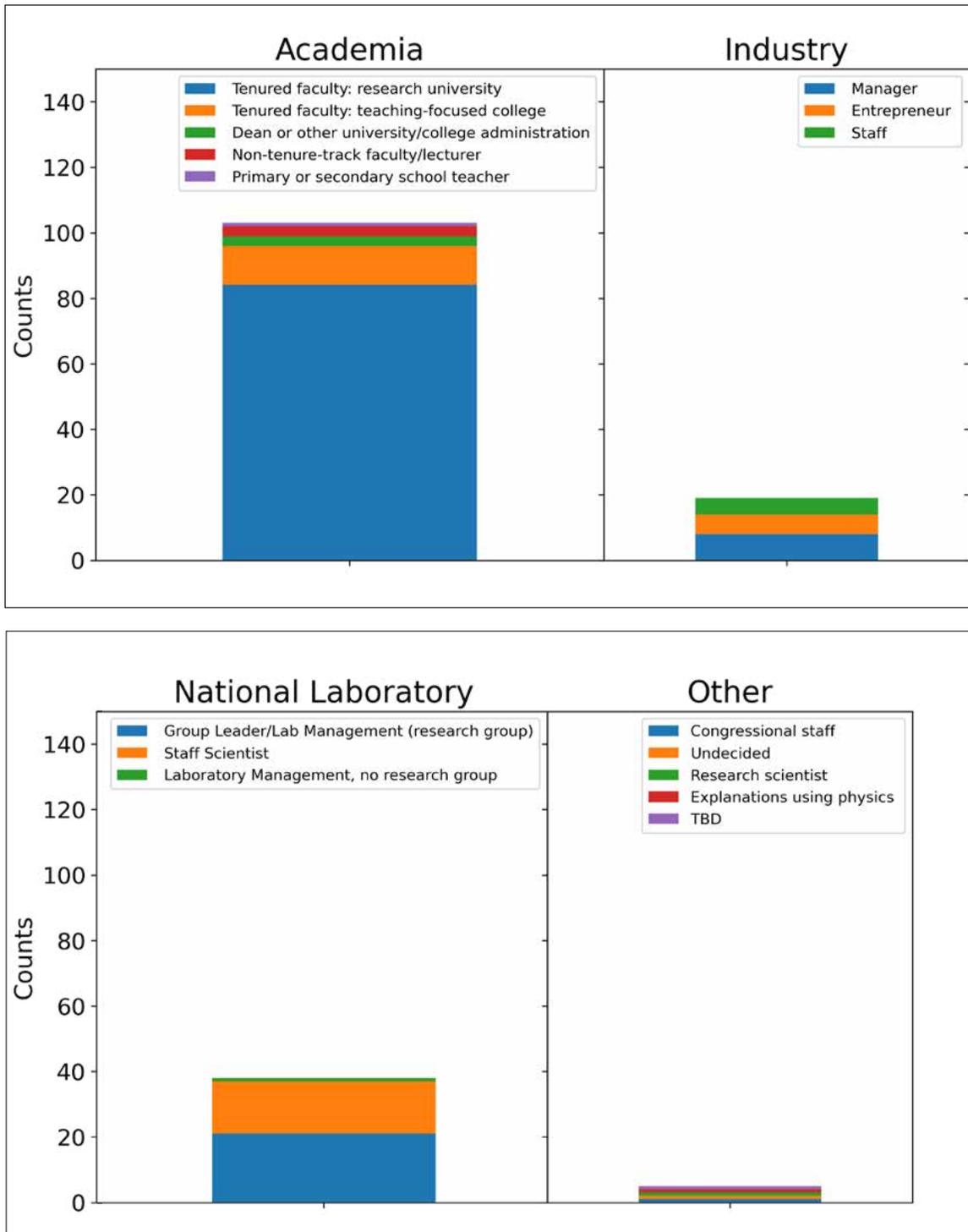
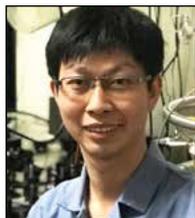


Figure 2: Breakdown of respondents in 2020 FECS survey for intended career goals or best guess. In the category "Other", we summarize the respondent's inputted answer.

# FECS 2021 Executive Committee on the Forum for Early Career Scientists



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Dr. Adam Iaizzi,  
Chair-Elect



Dr. Wennie Wang,  
Member-at-Large



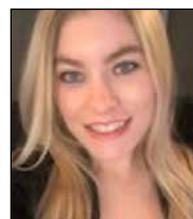
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