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TOP TEN TRENDS DRIVING SCIENCE

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Intro

WHAT ARE THE TRENDS DRIVING SCIENCE?

Some experiments might take place in a vacuum, but science never does. The pursuit of knowledge only happens within the context of the wider world. Research is not driven by pure, idle curiosity. Social, political, and economic trends influence every area of our lives, including the questions we ask and the work we do to answer those questions.

That doesn't mean scientists must bend to the will of the world. Often, the course of scientific research is shaped in opposition to a larger societal trend. But as we shape the world, the world also shapes us. Scientists must understand the forces affecting their profession if they wish to remain in the vanguard of progress. To ignore the tide is to be swept away.

This report is an introduction to 10 of the biggest ideas affecting scientists today. The trends listed here and their order where determined via a survey of 17 editors of ACS Publications journals. The editors who completed the survey ranked their picks for the most important social, political and economic trends affecting research in 2016. Once their rankings were tallied, a clear consensus emerged. Their list of topics includes new wrinkles in enduring issues, such as the search for research funding and science's place in society. But there are newer ideas too, such as globalization, open access, and other changes to scientific publishing in the 21st century. Each brings unique challenges, and maybe even opportunities for researchers who know where to look for them.

As you read through this report, you'll notice many of these trends are closely linked. It's hard to talk about how science is communicated to the public without mentioning climate change. Discussions about the future of scientific publishing are inextricably tied to topics such as open access, collaboration, and globalization. In many ways, the themes mentioned here are different aspects of a single master trend: Scientists adapting to thrive in a rapidly changing world.

Of course, a list like this can never truly be definitive. Depending on your field of study, your career path, or your location, other concerns might seem more pressing to you. I invite you to share your alternative takes on the most important trends in science with us via email at *axial@acs.org* or by visiting the ACS Axial blog at *www.axial.acs.org* and commenting on the posts associated with this report. We can't wait to hear what you have to say.

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RESEARCH BECOMES A TEAM SPORT

Once upon a time, collaborating on a paper meant meeting a colleague face-to-face and comparing research notes. This often meant traveling some distance, usually to a conference, to bring the collaboration to fruition. Now, you never have to meet your collaborator in person. With video chat options like Skype and FaceTime, the only condition for "meeting" someone is a reliable Internet connection.

The interdisciplinary nature of science and chemistry in particular encourage collaboration—and sometimes practically mandate it. "The moment the solution to a problem has societal relevance, it is no longer acceptable to restrict the tools used to find the answer to a single field," says Kai Rossen, Editor-in-Chief of *Organic Process Research & Development*.

One of the clearest signs of this trend is in the increase in the number of coauthors on papers. Papers with large numbers of coauthors are increasingly common, with the number of papers sporting more than 50 coauthors increasing from about 200 a year in 1990 to about 1,400 in 2014.[1] A paper on the Higgs boson may well hold the gold medal for most collaborators, with more than 5,000 participants[2]. But with increased collaboration becoming the new normal that record may not stand for long.

These papers are fantastic contributions to the scholarly record and could not have been achieved without contributions from throughout the global scientific community. Collaboration isn't just about efficiency. It's also about bringing a wide variety of expertise to bear on a problem, making it possible to discover solutions no one could have envisioned before. "Expanding classical organic chemistry tools with chemical engineering is highly enabling—and thus beneficial—as it will result in better solutions that will benefit society," Rosen adds.

Funding concerns are also a reason for collaboration. Research funding is competitive. More participants can mean a diversity of funds and a greater likelihood that the research will be completed. At ACS Publications journal, the average paper has funding from two sources. This pooling of resources provides better value to funders and prevents duplication of effort. This is especially important in countries where researchers receive government funding. Being able to show efficiency in the research process helps justify the public expense.

The opportunities for collaboration don't stop with publication. Scholarly communication networks help researchers share and discuss their work with others. Companies such as Kudos help authors share their work's implications in simple terms with the general public and media, while FigShare helps authors share their supporting information freely, including datasets that can help avoid duplicating work.

Despite its benefits, collaboration can present new challenges to authors. Scientists may need a wider base of knowledge to be able to work effectively with peers in other disciplines. They may face ethical issues surrounding who gets to take credit for discoveries or blame for errors. If your paper has hundreds or even thousands of coauthors, how will you decide what order to credit them in?

About 35% of all research published in 2010 was the result of international collaboration[3]. This means research will have to contend with logistical challenges as well. You might no longer have to get on an airplane to meet your co-author, but you may have to have a difficult talk about who needs to get on Skype for a 6 a.m. meeting to compensate for different time zones. Scientists will have to develop new skills, tools and work habits to get the most from these collaboration opportunities.

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SCIENCE IN A SKEPTICAL SOCIETY

Scientists have always challenged the public with new ideas, but sometimes it takes a while for a scientific finding to find broad public support. Research shows even trained scientists have to battle a subconscious level of uncertainty when presented with a true but counterintuitive statement.[4] But with persistence, even once-unthinkable ideas can gain wide acceptance.

Recently, however, we've seen a flurry of intense skepticism around ideas that were once uncontroversial, such as the safety of vaccines and fluoridated water, especially in the U.S. Old fights on subjects such as evolution and climate change seem to have a new intensity. "Unfortunately, many in society do not trust the opinions of scientists in important areas. For example, the notions that vaccines cause autism, or choosing to ignore the impact of human activity on climate change, to name a few. This leads to less enthusiasm for the funding of science," says *Journal of Chemical Information and Modeling* Editor-in-Chief Kenneth Merz.

The good news is there's little evidence to suggest a widespread, catastrophic decline in public trust in science in recent years.[5] Almost 4-in-5 Americans say science improves their lives. The bad news is that while Americans say they have positive views of science and scientists, they often say they won't accept certain scientific findings. Many Americans express sharply divergent views from scientists on topics such as climate science, the safety of genetically modified foods and human evolution.[6]

It's tempting to blame this on a lack of education. Surveys suggest both the public and scientists harbor dim views of U.S. education in science and math. But U.S. primary and secondary science education performs better than many people expect in international science education rankings.[7] Scientists continue to have high regard for post-secondary science education at U.S. institutions. "The U.S. is recognized as a leader at the college and graduate level," says Norbert Pienta, Editor-in-Chief of the *Journal of Chemical Education.*

But additional education doesn't appear to improve matters. In some cases, a high level of education correlates with mistrusting scientists around a particular issue.

Political and religious views, however, may impact a person's views on science, though no one factor is a sure indicator of this.[8]

"On issues such as climate change, many in the world (especially in the U.S.) are choosing to ignore or deny data and verifiable facts in favor of deeply held beliefs of a wishful or magical nature (in the sense that they are not or cannot ultimately be backed up by tangible data). To the degree that public policy is influenced by wishful and magical thinking that is contrary to verifiable facts, we abandon the potential fruit of science to help shape a better world. Don't get me wrong—I am not talking here about religion—whose interests are often well-aligned with science.
I am talking about willful know-nothingness that evades or denies facts based on a political or social agenda," said Charles Sanders, Interim Editor of *Biochemistry.*

While the number of people with a political or religious objection to a scientific finding may be comparatively small, their attacks may exact a disproportionate toll. "Politically motivated 'attacks' on science research are taking a toll on the positive public perception of university-performed science research, especially in some scientific disciplines," says *Analytical Chemistry* Editor-in-Chief Jonathan Sweedler. "Scientists need to spend their valuable time to ensure the informed dissemination of their scientific results in the media," says *Analytical Chemistry* Editor-in-Chief Jonathan Sweedler.

> Politically motivated 'attacks' on science research are taking a toll on the positive public perception of university-performed science research.

Europeans express high levels of enthusiasm for science as a force for good in the world. But religious concerns about science persist, especially in southern Europe. Almost 4-in-10 European Union citizens say society relies too much on science and not enough on faith. The same survey finds 60% of EU citizens say the world is changing too quickly and almost three-quarters say they're concerned about unforeseen side effects of scientific progress.[9]

In China, government support for research funding is strong.[10] A majority of students surveyed express an interest in pursuing a career in science and technology.[11] Research shows the Chinese are among the most likely to accept findings on evolution.[12] Yet alternative medical practices based on tradition continue to flourish there.[13] When it comes to climate change, both China and

India lag behind other major carbon-emitting nations regarding awareness and concern about the effects of climate change.[14]

In India, attitudes toward science can be somewhat stratified. More than 1-in-4 Indian citizens are illiterate.[15] These illiterate citizens are much less likely to know basic scientific principles and report high rates of acceptance of folk beliefs than citizens who can read. They are also less likely to feel that science improves their quality of life.[16]

International comparisons on this issue are difficult to make, as no universal survey exists to measure shifting attitudes on a global scale. It would be a mistake to look at some societies as more "scientific" than others. There are no purely evidence-based societies. The particular issues that are controversial may vary from place to place, but the idea that science can be controversial does not. Yet surveys from around the world reveal a healthy regard for science and scientists, even when people struggle with certain scientific findings.

Regardless of the nation, it is important to remember that popular skepticism toward science is not new. What is new is the ability of like-minded deniers to organize online, and to be fueled by those with a vested interest in denying the truth.[17] In the face of these challenges, scientists must do more than just discover the truth. They must be advocates for truth in an increasingly skeptical world.

8 BUT CAN YOU EXPLAIN IT TO YOUR PARENTS?

The landscape in which science communication takes place is changing.[18] Information spreads faster. It's easier for a finding to become distorted. If a finding proves controversial, opposition can spring up in a flash. Scientists may get questions or criticisms via social media. They may discover bloggers they've never spoken with are writing about their work with varying levels of accuracy.[19]

The alternative may be just as dire. Imagine unveiling your findings to utter silence. No citations. No media coverage. No reactions. Now imagine watching a colleague achieve all of those things, due to their ability to engage an audience and articulate the value of their work.

Communication is at the heart of many of the biggest challenges facing scientists today. Being able to articulate your work to a broad audience can have a tremendous impact on the discoverability of your research and the trajectory of your career. "Can you explain this topic to your mom? Your senator? If so, you have an automatic boost to your research," says Cynthia Burrows, Editor-in-Chief of *Accounts of Chemical Research*.

But science communication isn't just about you. It's about the future of science.[20]

Researchers' ability to explain their work and its importance will influence what kinds of projects are funded. Researchers' testimony can affect the kinds of laws and regulations put in place. Most importantly, being able to explain the impact of your research can help shape the public perception of science and even change people's lives.[21] "We, as scientists, need to address this issue and become better at framing the importance of scientific research in the modern world," says *Journal of Chemical Information and Modeling* Editor-in-Chief Kenneth Merz.

Scientists need to demonstrate their competency, but also show warmth.

The best practices around science communication have evolved. It's not just about sharing information and correcting erroneous beliefs.[22] The psychology of skepticism is complex. Exposing a person to new information may do little to weaken their resolve and can even strengthen their opposition.[23]

Instead, scientists need to demonstrate their competency, but also show warmth. Scientists are often ranked highly for the first trait, but not the second, which can limit their ability to influence others.[24] Whether talking to reporters or to the general public, scientists must be aware of their audience's perspective. Scientists tend to have specialized knowledge and a rigorous focus on research details that their audience most likely does not share. They must find ways to bridge the gap between those worldviews.[25]

This requires finding a balance between explaining research in an accessible way and running the risk of sensationalizing or otherwise distorting research. It also requires not resorting to a paternalistic attitude.[26] Many of the best practices of science communication are easy to understand. Avoid jargon. Talk about why a finding matters, rather than the methodology used. Put research in context. But the application of these ideas is nuanced and can only be mastered with practice. Which terms count as jargon? The answer may well depend on the audience.[27]

By engaging a variety of different audiences on a regular basis, scientists can learn to calibrate their explanations. Not only should scientists seek out venues for informal science communication, they should evaluate their performance so that they can refine their approaches. Science communication, much like scientific research, may require much trial and error before a breakthrough is made.

KNOWLEDGE KNOWS NO NATION

There was a day when science was dominated by researchers from Europe and North America. That day is not today. Just as science has become more open and collaborative, it has also become more global. Consider that while we might be called the American Chemical Society, two-thirds of our readers and authors are based outside the U.S. In the past five years, we've published 48,000 papers from Brazil, India, China, and South Korea. Our journals have 48 Associate Editors and 228 Editorial Advisory Board Members from those countries.

What's true at ACS is true all over the world. We're seeing a rapid rise in scientific output from the Middle East, China, and India, among other regions. As more nations prioritize science, the reach of research increases. Governments are focusing on scientific output and prioritizing contributions to the scholarly record. This means more voices, more ideas, and more innovation. "The strengthening of science throughout the world, especially in China and India, will have a long-term impact on all fields of science," says Sharon Hammes-Schiffer, Editor-in-Chief of *Chemical Reviews*.

Take a closer look at China, which spent 2% of its gross domestic product on research and development in 2014, surpassing the EU's spending levels as a share of GPD for the first time. The EU's 28 member nations spent a combined $334 billion that year, compared China's $345 billion. China's total may be well short of the $433 billion the U.S. spent in 2013. But U.S. spending has hovered between 2.5% and 2.7% of GDP since 2000, while China's has increased steadily from 0.9% to more than 2% today.[28] If China's recent increase in research funding is ongoing, it could someday surpass U.S. research funding in raw dollars. China's investments have global significance, as funding on that level attracts scientists from around the world.

Historically, very little of China's research and development spending is invested in basic research. Instead, most funds go toward development of commercially focused technology, developments that could help China economically and socially. Sustainable energy, for example, is an area toward which the country's government directs significant investment.[29] There are signs, however, that this may be shifting. "The Chinese government has paid much more attention to fundamental science and has set up funding institutions to support scientists," said Dongyuan Zhao, Ph.D., professor of chemistry at Fudan University in Shanghai and senior editor of *ACS Central Science*.

China isn't the only country rapidly becoming a scientific powerhouse. In 2014, India became the first country to reach Mars on its initial attempt.[30] India's politicians are resolutely supporting these scientific endeavors. During his first year in office, India's Prime Minister Narendra Modi launched a determined plan to make India a leader in solar power.[31]

Investments in places such as China and India may have effects beyond their borders. In the U.S., for example, some politicians see increased scientific funding abroad as a challenge and are using the issue to agitate for more funding at home. Increased competition in the marketplace of ideas may act as a guard against complacency and make supporting science a matter of pride for every nation.[32]

The U.S. continues to attract about 1.2 million international students, including about 500,000 in masters or doctoral programs. About 40% of international students are pursuing STEM education, including 82% of all students from India and 39% of all students from China, compared with 19% of European students.[33] Yet that figure may be stagnating, as more students opt to go to school in countries with less stringent immigration laws.[34]

An increase in research funding in some parts of the world throws other areas into sharp relief. In spite of rapid economic growth, many nations in Sub-Saharan Africa still lack research infrastructure and support. These disparities present challenges for both local governments and international bodies to ensure brilliant minds in certain parts of the world aren't left behind.[35]

In the future, a researcher's country of origin may become a purely circumstantial detail, and local funding and political support may begin to matter less. Already, once-regional conferences are now attracting people from all over the world. Video conferencing programs have opened up the doors for global collaborations. Scientific organizations vie for an ever-more global audience. Science has always transcended borders. Increasingly, researchers can too.

OPEN ACCESS IS EVERYWHERE

Allowing scientific research to be freely available is increasingly important for many researchers and funding organizations. The thought is that if research is freely available, it can be built upon with ease and used to further scientific discovery. These breakthroughs, in turn, can lead to economic and social improvements that will better society.

"[Open access] will become the standard. It already seems to be in Europe," says *Journal of Chemical Theory and Computation* Co-Editor-in-Chief William Jorgensen. The European Union took center stage on this issue with its mandate that by 2020, all scientific articles using public or public-private funds in Europe must be freely available.[36] Many European funders and institutions have been issuing their own mandates regarding open access, but until now they were not converging around one model.

In the U.S., the public access policy of the National Institutes of Health (NIH), one of the country's largest funding agencies, is widely known. It requires all research published with NIH funds to be made publicly available in 12 months or less on PubMed.[37] Effective April 2008, this was the first policy in the U.S. to mandate some form of open access on a large scale. Many other funding agencies followed suit. By tying funding to open access requirements, these organizations have helped make open access the de-facto standard for researchers in many fields. Open access in the U.S. is converging around the 12-month model, with some notable exceptions, which requires immediate open access under a CC-BY license.[38] U.S. publishers, including ACS journals, offer a variety open access options to fit researchers' needs, including making articles open access upon publication.

In Latin America, the partnership between the research network ScienceOpen and the Scientific Electronic Library Online (SciELO) is a notable development. The partnership will fully integrate content from the two sources for a more global perspective on the scientific literature. All SciELO content is universally accessible for free in an open access, full-text format. With the inclusion of SciELO, ScienceOpen now contains more than 2.2 million open access articles. ScienceOpen will also have more than 15 million article records upon full integration.

Why is this happening now? Technology is one factor. Infrastructure for open access transaction models is becoming more robust, making open access quicker, simpler, and easier to measure. Funders realize this and are increasing mandates on any research published with their funds to be made freely available so it can have a wider impact. Openness also means that results can be tracked with greater precision. Funders can use these insights to learn which research is most relevant and make better funding decisions in the future.[39]

Researcher attitudes toward open access publishing may also be changing. The initial surge of for-profit open access publishing created a wave of low-quality journals that would publish anything for a price. [40] But now the field includes many not-for-profit publishers with a different set of motives, which have helped the sector grow to more than 4.3% of the scientific, technical, and medical journal publications market as of 2014. [41]

Publishers and others are developing tools both for funders and authors to make open access research more sustainable. Researchers now must determine who will pay the article processing charges for open access. Is it the author, the funder, or the author's institution? They also need to know the optimal license to publish under to meet all funder requirements. Funders, on the other hand, need to be able to track payments and measure the impact of the research they fund. New models and tools have sprung up to meet these needs and more are doubtless on the way.

An example of this is FundRef, a common tool employed by ACS Publications and other publishers. FundRef allows the corresponding author to report their funders during the submission process. If an article is accepted, the author will automatically be emailed with reminders of the funder's requirements and what publisher open access licenses will meet these requirements. This helps perpetuate the cycle of open access, ensuring a funder's needs are met and researchers can continue to benefit.

The problems with open access, including sustainability and misuse of content, are still very real. But the conversation has now shifted. People are no longer asking "Is open access necessary?" but rather "How do we deal with issues within current open access models?" For those who believe science should be open, that's significant progress.

5

THE FIGHT FOR FUNDING

As long as there have been scientists, there have been scientists in need of research funding. The online archives of ACS journals contain references to the need for funding going back 90 years[42], but of course the problem is even older than that. Historically, researchers were limited to getting funds from their personal contacts and wealthy patrons. Alexander Graham Bell's work on the telephone was financed in part by money from the father of one of his students. But beginning in Germany in the 19th century, government-funded universities began supporting research directly. After World War II, the U.S. created a number of research-focused offices, such as the National Science Foundation and the National Institutes of Health. Public funding joined universities and corporations as one of the major drivers of research.[43] So why list the search for funding as one of the leading trends in science in 2016?

First, money is an enduring concern for scientists everywhere. Even if every other item on this list becomes irrelevant, scientists will still need to find a means of supporting their work. As Cynthia Burrows, Editor-in-Chief of *Accounts of Chemical Research* reminds us, "Money makes the world go round." Even if in the face of a public health crisis, such as recent outbreaks of Zika virus, scientists need to find a way to pay for their research. Sometimes, that funding can still be held up by issues that have nothing to do with science, such as political concerns.[44]

Second, the way funding is being apportioned to researchers today is changing. As new fields gain prominence, it can be harder for established disciplines to find the same level of backing they had in the past.[45] Scientists aren't immune to the human inclination to chase trends. Even if they were, people who aren't scientists are involved in making funding decisions. Researchers may feel pressure to focus their work on fields that are easier to fund, rather than chasing after what they know to be more important questions, especially as state-funded research

Scientists aren't immune to the human inclination to chase trends.

grants become scarcer. Even researchers in prominent fields may feel the need to transition to a career outside the lab if they can't secure funding[46].

Scientists engaged in basic research face some of the most difficult challenges in securing funding. It's easier for organizations, both public and private, to say yes to research aimed at fixing a specific problem. Public funding for basic research is meant to alleviate this concern, but politicians may look to score points with their constituents by mocking research they see as frivolous. "With many governments feeling they need to justify spending on education and research, the shift in focus to applied science over fundamental science in many countries is a major concern for the advancement of knowledge," says *ACS Sensors* Editor-in-Chief Justin Gooding.

But the news isn't entirely bad. In the U.S., 2016 brought an increase to federal funding for research through the National Institutes of Health, The Department of Energy's Office of Science, and The National Science Foundation, following years of stagnation. At the same time, legislators made the federal research and development tax credit permanent, following more than 30 years of temporary extensions.

This move may give private organizations the additional financial security they need to make long-term research commitments.

In China, government research funding increased by 23% in the decade leading up to 2014. Government funding has traditionally gone to applied science projects, often with grand goals attached such as nuclear power and space exploration. Funding for basic research has increased in recent years[47], however, and researchers are increasingly receiving more control over how their funding is spent.[48]

At the same time, other sources of funding are appearing. Patient advocacy groups can help fund research into rare diseases. Crowd-funding sites can help startups raise capital or even be used to fund research directly.[49] These options offer welcome additional funding sources for researchers, but they also present a dilemma. These kinds of options work best for research into applied topics that are either easily understood or that have deep appeal for a particular group, such as patients with a particular disease. Democratic funding may not be a tide that lifts all boats.

More troubling is the possibility that funding shortages may dissuade bright, capable individuals from pursuing careers in research. "Being a professor is fun and rewarding. However, funding trends (and perhaps more than funding trends, a perception of decreased funding) are discouraging many qualified individuals from pursuing this career path," says *Analytical Chemistry* Editor-in-Chief Jonathan Sweedler.

At the same time, science is becoming an ever-more international pursuit.[50] More researchers are looking to international businesses or research consortia to fund their work. This encourages collaboration and crosspollination. It also means that skilled researchers don't have to make do with mediocre local funding sources. As a consequence, nations that don't prioritize public funding for research place themselves at risk of losing some of their brightest minds.[51]

4

PUBLISHERS LOOK IN THE MIRROR

What exactly is a scientific publisher in 2016? Are we information aggregators? Content-related product providers? Content quality checkers? Twenty years ago, the definition was much simpler: Scientific publishers vetted submitted manuscripts, formatted them for publication, and then handled the distribution of journals. Today, publishers have to rethink their roles to remain relevant. Publishing is still about processing and delivering information, but now the emphasis is on different parts of the process.

"There is a lot of discussion on the validity of claims made in scientific papers. Many are retracted based on fraudulent practice or manipulated data," notes Prashant Kamat, Editor-in-Chief of ACS Energy Letters. Peer review remains a critical function, especially with the rise of open access publishing. It is the publisher's job to not only communicate research to the scientific community, but also to make sure that research is of the highest quality and free from manipulation and plagiarism.

The number of retractions for papers indexed by Thomson Reuters' Web of Science increased from about 30 per year in the early 2000s to about 400 in 2011, an increase of about 1200% compared with a 44% increase in papers published. Retractions total about 0.2% of all papers published in scholarly journals each year but high-profile retractions can undermine the credibility of a journal, a field or even the public perception of science writ large.[52] To keep up with submission increases, improvements to the peer review process are needed.

"With the incredible demands on our time and never-ending stream of review invitations, together with ever diminishing time until the review is due back to editors, it is now impractical to spend a long time reviewing papers," says Greg Scholes, Deputy Editor-in-Chief of *The Journal of Physical Chemistry Letters*. "The new skill is to write a helpful report in around 15 minutes. This trend suggests the question—do we need to rethink how to best implement peer review?"

A lack of reviewer education may be a part of the problem. A recent survey found that formal peer review education is scarce: 4% of respondents participated in a journal's reviewer mentoring program, 4% attended a workshop/seminar, 4% watched a video, and 2% watched a webinar. The survey found 77% of reviewers want further peer review training.[53]

Another area where publishers can play a unique role is in managing trends in research. Many researchers are becoming concerned about the pressure to pursue a trend. Publishers have to be the counterweight to scientific hype. At the same time, it falls to them to look out for new and exciting fields and to recognize great work no matter where it comes from. "A challenge for publishers is how work out how to select and communicate the best innovative new science across a diversity of topics, and taking some risk foreseeing papers that might be influential or seed new directions, rather than following trends," says Scholes.

Modern publishers provide resources for scientists on a variety of topics. They provide access to webinars, online tools, white papers, videos and more. They can also host conferences that provide researchers with a chance to get together and share ideas. Publishers can also act as intermediaries between the scientific community and the rest of the world, helping to improve the discoverability to important papers, as well as serving as a resource to help journalists deliver more accurate reports. "The news media likes to promote sensational news. People who hype their research claim to solve societal problems with lab scale experiments. For example, a catalyst that works for few minutes cannot solve world's energy problems," says Prashant Kamat, Editor-in-Chief of *ACS Energy Letters*. Publishers also have the power to help the general public and journalists alike to understand when a paper is being taken out of context.

Even though the technical barriers to sharing research have fallen in recent years, publishers are still a key part of how research is vetted, shared, and explained. The challenge that lies ahead is to find new ways to contribute to that process while adapting to the global forces remaking the research landscape.

Publishers have to be the counterweight to scientific hype.

3

SMALL IS BIG

Nanoscience is the study of materials' properties at sizes smaller than one billionth of a meter. Nanotechnology is the development of the ability to manipulate materials one atom or molecule at a time. Together, these two disciplines make up one of the most buzzed-about topics in all of science. Across the globe, scientists are betting that small materials will have big impacts in the near future.[54]

Nanoscience offers "significant promise for future advances in problems related to energy, the environment, and biology," says *ACS Applied Materials & Interfaces* Editor-in-Chief Kirk Schanze.

At the same time, nanodisciplines are often misrepresented. Based on popular news articles, you'd be forgiven for assuming that nanoscience is a new field, filled with virtually limitless potential. In truth, formal nanoscience is at least 150 years old and it's far from a unitary discipline. Nanoscience is a part of a wide variety of fields, depending on the application. Interesting nanoresearch is being done in subjects as diverse as agriculture, biology, engineering, materials, medicine, physics, photonics, regulation, toxicology, and many more besides.

"The explosion of research on nanoscale artificial photonic motifs comprising plasmonics, metamaterials, and metasurfaces has allowed the ability to sculpt the flow of light and heat in materials at the nanoscale and in ways not possible with natural materials," says *ACS Photonics* Editor-in-Chief Harry Atwater.

If the ideas behind nanoscience are nothing new, then why is nanoresearch having such a surge in activity? Some limited studies of the properties of nanoparticles were possible in the 19th century, but we've only developed the tools needed to manipulate materials at nanoscale in the last few decades. Nanotechnology was made possible in the 1980s, with the development of advanced microscopes that made it possible to manipulate a substance one molecule at a time. In the 21st century, new tools have allowed scientists to begin to put theory into practice in ways that generate headlines.

"Experimental and computational tools are now at a point where new materials can be designed via modification of an existing scaffold or the design of novel scaffolds from the ground up. This will afford new structural and catalytic materials that will be able to address contemporary issues in catalysis, energy conversion, energy storage, etc.," says *Journal of Chemical Information and Modeling* Editor-in-Chief Kenneth Merz.

Now applications of nanotechnology are turning up in a variety of fields. Some of the most interesting applications are in the medical world, where nanoparticles could someday be used for everything from testing to targeted delivery of medicine. This is a particularly interesting application in cancer treatments, where the side effects of chemotherapy drugs can often be nearly as devastating as the disease they seek to treat. “I feel that with the rise of nanomedicine, nanoparticles for both diagnostics and drug delivery and going to continue to become more and more important,” says Justin Gooding, Editor-in-Chief of *ACS Sensors*.

At the same time, the ability to co-engineer nanomaterials and biomolecules is opening up new doors for biological researchers. “After many years of creating nanosystems that can interact with proteins and nucleic acids, researchers are finding new ways to co-engineer these systems to obtain new synergies, applications, and sometimes even emergent properties,” says *Bioconjugate Chemistry* Editor-in-Chief Vincent Rotello.

The potential of nanoscience and nanotechnology are is very high. Unfortunately, the hype surrounding the field is every bit as great.[55] Advocates for nano-related research should fuel interest in the field by trumpeting the real-world advances made possible by nanotechnology, such as smartphones. At the same time, they must work to temper science fiction-fueled-expectations that nanotechnologies will solve every problem in the near future.[56]

2

BIG DATA IS MORE ESSENTIAL THAN EVER

Research has always meant data, but never quite like this. Modern research produces experimental data not just from *in vitro* and *in vivo* studies, but also from simulation-driven *in silico* work. The ability to interpret, compare, and contrast data sets is essential.

As the amount of scientific data increases, it becomes imperative to determine how to store it, archive it, and make it accessible to other researchers and the general public. This openness can have enormous benefits. For example, in medicinal chemistry, data analysis can aid in decision-making for drug discovery research.

This is motivated by parallel synthesis, the creation of increasingly large and complex analytical and biological data sets associated with each new chemical entity and the requirement to integrate publicly available information, including patent literature, into the design process. If other researchers can easily access this information, it can speed up the production of future research and avoid duplication.

Managing the data is a complex process, however, and it can require the use of specialized tools. Dealing with large data sets isn’t just about file size. It may also mean being able to keep up with evolving data sets or handling a combination of structured and unstructured data. Researchers also need the means to detect errors hidden in rows and rows of tables. These skills may be outside the traditional training of many scientists. In 2016, however,[57] every researcher needs to have at least some skills as a data scientist.

Using existing data sets makes sense. It can save researchers time and money and, when applied to their own work, can potentially aid in research decision-making.[58] “Potentially” is the key word here, because data is useless if the research community cannot learn how to effectively harness it. While researchers are great at producing data, they need better data management infrastructure, systems, and training. Organizations also need to find standardized ways of structuring data to allow researchers to use it more efficiently. According to one estimate, 40% of all research and design experiments are duplicated effort brought on by efficient design or a lack of information technology resources.[59]

“Conversion of massive amounts of chemical and biological data into cogent insights is becoming a significant area of opportunity. With ever-advancing sensor capabilities and the expanding power of computers to generate computational data the need to understand massive data sets will drive a lot of scientific endeavors and will offer exciting opportunities to advance the chemical and biological sciences,” says Kenneth Merz, Editor-In-Chief of the *Journal of Chemical Information and Modeling*.

This optimism is shared by many others including Jonathan Sweedler, Editor-in-Chief of *Analytical Chemistry.* “This is a golden age of measurement science. From the evolving challenges of environmental monitoring to following the chemical intricacies occurring in our brains that give rise to consciousness, analytical chemistry-related grand challenges are capturing national attention and becoming national research priorities.”

This rise in measurement science extends to all industries. And chemists are at the heart of many of these advancements. “Chemists have been central to these developments and will exploit genetic information in new and unexpected ways going forward. Links between genetic changes and their resultant human diseases increasingly will be understood in molecular terms, and new treatments and preventive strategies will emerge,” says Carolyn Bertozzi, Editor-in-Chief of *ACS Central Science*.

This is a golden age of measurement science.

How can we make it easier for researchers to keep having data-fueled discoveries? One answer is education. Scientists of all types need a solid grounding in data management. They should be able to recognize sources of relevant information, prepare raw data, use statistical tools, extract meaningful information, interpret results, recognize potential problems, and make visualizations to convey their findings. That kind of training is especially essential for reviewers and editors, who need to be able to spot false positives and statistical manipulation to prevent spurious studies from gaining traction.

Scientists have more information than ever at their disposal. But to do any good, they have to know how to use it.

CAN SCIENCE SAVE THE WORLD?

In late 2015, representatives from 185 countries met in Paris to commit to a framework for addressing climate change.[60] The accord was hailed as a historic victory, but even the deal's biggest supporters say a great deal of work remains.[61] The goals discussed in Paris are modest and the path to achieving them is unclear. It seems unlikely that politicians will save the planet by themselves. Fortunately, they won't have to.

Chemists have the opportunity to be the driving force in addressing anthropogenic climate change.[62] Conservation and regulation are essential to solving the climate crisis. But they're not enough in the face of population growth and rising standards of living. Chemistry helped build the modern world with its insatiable appetite for energy and dependence on fossil fuels. But if chemistry once helped contribute to the climate problem, it is now at the heart of our search for a solution.[63]

"We all know that people's demand for a high quality of life will continue to increase the global demand for energy," notes *ACS Central Science* Editor-in-Chief Carolyn Bertozzi. "We look to chemical reactions to provide energy and in turn to novel energy sources to power chemical reactions."

Addressing climate change tops this list of the most important issues in science for three reasons. First, climate change is a truly global problem. Second, developing an effective response to climate change will require contributions from a broad swath of scientific disciplines from around the world. Finally, as politicians, businesses, and consumers alike become more concerned about the issue, climate change is having a major impact on research funding and publishing. "The need to develop alternative energy sources is at a critical point and has economic, societal, and scientific implications," says Sharon Hammes-Schiffer, Editor-in-Chief of *Chemical Reviews*.

Climate change is often discussed as a single problem, but solving it will require a wide variety of solutions. Some areas already get a lot of attention. "Research efforts related to energy conversion and storage, as well as improving the efficiency of devices, will continue to provide a major research thrust," says Prashant Kamat, Editor-in-Chief of *ACS Energy Letters*.

"Research on solar materials and batteries is growing at an impressive clip," notes George Schatz, Editor-in-Chief of *The Journal of Physical Chemistry A, B,* and *C*.

But to effectively to effectively address climate change, we will also need to create better methods of removing greenhouse gases from our atmosphere and develop more complete understandings of the reactions taking place in our atmosphere and our oceans because of our changing climate.[64]

The seriousness of the problem, combined with the breadth of disciplines involved, will have a significant and lasting impact on research funding throughout the world.

"In the aftermath of the COP21 conference on climate in Paris, world leaders have committed themselves to 'Mission Innovation,' in which they develop plans to double scientific research in their countries aimed at mitigating climate change," explains Harry Atwater, Editor-in-Chief of *ACS Photonics*. "Each country is charged with developing its own plan and execution pathway. In the U.S., President Barack Obama has directed the Department of Energy to develop a plan to meet the Mission Innovation objective. says Harry Atwater, Editor-in-Chief of *ACS Photonics*. "Meanwhile, Bill Gates and other corporate leaders have founded the Breakthrough Energy Coalition to spur corporate and private investment of more than $1billion in scientific research funding related to sustainability science and technology. This will have profound effects on research directions for chemists and all physical scientists, who will be at the heart of this new initiative."

And what about fossil fuels? They'll still have a role to play, but an increased emphasis on renewable energy will mean we can reserve their use for other tasks. "Petroleum is so valuable as a commodity chemical for production of plastics—I cannot believe we are burning it for energy!" says Courtney Aldrich, Editor-in-Chief of *ACS Infectious Diseases*.

THE MOST IMPORTANT UNSOLVED PROBLEM IN CHEMISTRY

What's the most important unsolved problem in chemistry? It's a deceptively simple question. You could ask 100 different chemists and get 100 different answers. Chemistry is the central science, with ties to every other scientific discipline. It's only natural that someone studying physical chemistry would have a very different answer than a biochemistry researcher.

But just because there isn't a single correct answer doesn't mean the question isn't worth asking. Debates like this help us have larger conversations about the nature of progress, the value of knowledge, and the challenges faced by humanity. Plus, they can be a lot of fun.

In that spirit, we asked a dozen editors of ACS journals for their take on "the most important unsolved problem." Here are their answers.

"Understanding the complexity of systems in order to use chemistry to model natural biology."

Robin Rogers
Editor-in-Chief of *Crystal Growth & Design*

Prashant Kamat
Editor-in-Chief of *ACS Energy Letters*

"Why can't we design chemical systems more efficient than photosynthesis? We know how it works but we do not know how to build one! Despite the efforts of several decades, artificial photosynthesis has failed to replicate the chemistry of reaction center of photosynthesis. (Most of the claims made today do not address efficiency, selectivity, and stability issues that can lead to a practical device. If you disagree, show me a prototype reactor!"

"Development of energy-efficient, selective catalytic pathways for reduction of carbon dioxide."

Harry Atwater
Co-Editor-in-Chief of *ACS Photonics*

"The ability to accurately predict the structure of complex biological or synthetic macromolecules and to relate the molecular and supramolecular structures to properties and reactivity."

Kirk Schanze
Editor-in-Chief of *ACS Applied Materials & Interfaces*

"How to predict catalytic activity or new catalysts for organic transformations."

Greg Scholes
Deputy Editor-in-Chief of *The Journal of Physical Chemistry Letters*

"Health-related issues including cancer, neurological disorders, and drug toxicity."

William Jorgensen
Co-Editor-in-Chief of *Journal of Chemical Theory and Computation*

"We are still not able to prepare complex organic molecules well. The general perception and the message coming from many organic chemists is that organic chemistry can make everything, the definition of success being the preparation of a minute amount of a compound after a massive investment of resources. This mismatch between necessary investment of resources and outcome clearly points to the fact that the organic community is still very far from making it possible to prepare complicated molecules easily. There is a huge need for a great improvement, probably combining new strategies with new methods, often catalytic, but also adding engineering aspects and learning from biology."

Kai Rossen, Editor-in-Chief of *Organic Process Research & Development*

"Most important: energy. Most fascinating: prebiotic chemistry."

Cynthia Burrows
Editor-in-Chief of *Accounts of Chemical Research*

"Efficient water purification worldwide."

Sharon Hammes-Schiffer
Editor-in-Chief of *Chemical Reviews*

"Biochemistry on earth is based on abundant water being available, hydrocarbon-based biochemistry, and temperatures in the vicinity of 300 K, plus or minus 50 degrees. Could there be life forms in the universe that are based on radically different chemistry than the biochemistry of earth and that might thrive under conditions far more "extreme" than even the most extreme conditions supporting life on earth?"

Charles Sanders, Interim Editor of *Biochemistry*

"What is the chemical nature of memory and thought? While it's a long-standing question reaching back to Aristotle, advances in microscopic and chemical measurements of the brain will allow us to answer this longstanding question in the coming decade."

Jonathan Sweedler,
Editor-in-Chief of *Analytical Chemistry*

"How to assemble complex, hierarchical materials from molecular building blocks as nature does. Related is how to predict from molecular building blocks a final material and its shape."

J. Justin Gooding
Editor-in-Chief of *ACS Sensors*

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