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EDITORIAL

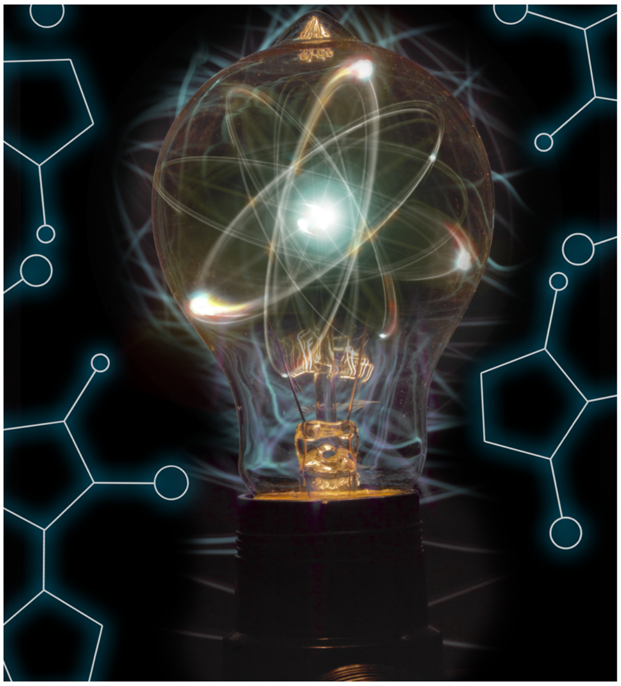
Grand Challenges in Chemistry for 2016 and Beyond

When several *ACS Central Science* Editors met for dinner at the 2015 Pacifichem meeting, conversation turned to the grand challenges facing science and society, and those we felt chemistry was in a unique position to solve. With the New Year, we thought we would share our ideas in our first editorial of 2016. The arenas in which we see chemistry having the largest influence are the molecular bases of disease and aging, alternative energy advancement, and the conservation of our elemental resources.

The first challenge we identified is often hidden under the guise of an information problem. Routine access to genetic information is changing profoundly how we think about the molecular sciences and their role in society. Substantial information about one's own genome can be obtained in a few weeks for several hundred dollars, while whole-genome sequencing is available to anyone willing to spend a couple thousand. At the same time, powerful new methods of genome editing, still under active development, are raising important questions about what kinds of experiments should, should not, or "must" be done.

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. New chemical tools will allow us to probe genome organization and gene regulation with greater specificity and resolution, and provide a basis for deeper understanding of evolution, the microbial world, developmental biology, neuroscience, and the mechanisms by which the immune system distinguishes self from non-self. Perhaps just as importantly, access to personal genetic information and open discussion of the ethical issues raised by personalized sequencing and genome editing technologies will provide new windows for nonscientists into the nature and value of the scientific enterprise.

A corollary to chemistry's central role in leading us from genetic signatures to medicines will be its key to understanding what it means to be healthy across all ages—something not predicated on genetics alone, as twin studies have shown time and time again. In our youth, we count on the development of a healthy microbiome for proper immune function. Defining the molecular basis of interspecies communication in our guts, respiratory tracts, and skin is a major challenge for chemists, with profound implications for new avenues to improve health. As well, the chemical basis of aging is a fascinating and wide-open field with the capacity to spawn the development of new analytical methods to address the problem at many hierarchical levels. Aging occurs at the level of molecules, cells, tissues, and multiorgan systems, and the program is far from understood at a molecular level. Biomarkers of aging are in high demand and would help in formulating interventions that might prolong our health span, an especially important goal in an aging society with high health care economic burdens.



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We all know that people's demand for a high quality of life will continue to increase the global demand for energy. We look to chemical reactions to provide energy and in turn to

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novel energy sources to power chemical reactions. Further, chemistry holds the key to controlling energy transfer between renewable sources and our existing infrastructure, while simultaneously exploring new sources of energy to meet the needs of social development and human progress. These transformations will inevitably bring new environmental problems. Air pollution prevention and water treatment both require new chemical processes and materials (nanomaterials, 2D materials) as well as new energy sources. Finally, sustainable energy, such as water photolysis hydrogen production, solar energy utilization, and CO_2 capture and transformation, depends on the understanding of energy chemistry. From using modern imaging techniques to attacking basic problems of photochemistry, electrochemistry, magnetic chemistry, and catalysis chemistry, these tools will improve the efficiency of energy conversion, and balance our needs for energy with protecting the environment.

Beyond the much discussed global carbon cycle and issues of energy and climate change, the Periodic Table provides a chemical blueprint for all life on our planet and our surrounding environment, and human activities impact that blueprint from the nitrogen cycle for food production to the need for rare earths and other metals for technological applications and medicines. The recent addition of 4 new members to the Periodic Table shows that this blueprint is living and even expanding. Because under ambient conditions elements are neither created nor destroyed, a major challenge for chemistry moving forward with a growing and increasingly industrialized population is, how do we best use our resources of elements with minimal perturbation on the environment?

In the biological arena we ask, can we create or find receptors to selectively recognize these elements in the environment or in our bodies? We are already on our way to being able to image every single molecule in the cell, the basic building block of life. From a more traditional synthetic organic perspective, can we develop methods to specifically make and/or break bonds between any and all elements in the Periodic Table? Synthetic chemistry requires the utilization and/or manipulation of free energy. Current organic chemistry strategy often instinctively (or explicitly) teaches disconnection to petroleum-derived feedstocks and hence (either theoretically or practically) "spends" free energy that was ultimately harvested from the sun eons ago. A truly renewable approach would instead try to restrict itself to the use of molecules as feedstocks that represent the small fraction of "sun-derived" free energy (our most inexhaustible energetic resource) that is trapped *now*.

This might, in turn, be underpinned by, for example, agrochemicals or light-harvesting molecules that could potentiate this utilization in a manner that "paid back" more than was required to make them. Providing any accompanying drain on other global resources (e.g., water, space) were nonprohibitive, such a molecule would thus provide an "amplified" source for its own synthesis while also allowing us to marshal more of the molecules on this planet in the collection of a greater fraction of this "solar harvest".

Lastly, we expect computational tools to continue to enable more accurate visualization and modeling of these and many more problems as they have already led to major discoveries in chemistry. Studies thus far have concentrated on solving a problem on a single time and length scale. There are multiple challenges to enable modeling of larger-scale systems and to investigate phenomena at multiple scales.

Quantum simulations such as density functional theory (DFT) are limited to small systems and short dynamical trajectories. Mesoscale studies require simulations that accurately describe long-range interactions, including dispersion forces via improved functionals. Quantum simulations should provide accurate force fields capable of proving multiscale modeling. Combining quantum information with atomistic molecular dynamics simulations will enable the study of complex systems where chemical reactions take place.

Atomistic simulations elucidate the roles that molecular components play in a system and enable the design of materials with targeted macroscopic properties. To get to these insights, we must develop classical force fields to accurately model polarizability and chemical reactions. From there, we will be able to describe systems with charged components and to describe nonequilibrium phenomena in systems where bond breaking and formation occur.

One truly beautiful thing about chemistry as the central science is that findings in any of these arenas will influence and change how we see and approach each of the other challenges, and reveal a rich variety of new ones. Let us know the grand challenges you are working on in the New Year. We want to publish your advances on these and other key problems in *ACS Central Science*.

The journal is already proving both a strong and unique venue to highlight your best research findings. From complimentary *ACS AuthorChoice* open access licenses to distribute your best work around the world to engaging Center Stage interviews and The Hub news stories by colleagues at *C&EN*, we showcase your research to a wide,

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global audience. We've added commentary from first-class scientists to put your work in a broader context, and produce embargoed press releases with the ACS Office of Public Affairs on many research articles. In fact, more than half of published articles in 2015 received outside press including stories featured in *C&EN*, *Forbes*, and *The Daily Mail*.

As researchers ourselves, we value your time and focus on a peer review process that is objective, fast and fair. Making quick initial decisions and avoiding the Mobius strip of the revision cycle helps us achieve the fastest times from submission to publication amongst leading multidisciplinary journals—around 9 weeks. We are proud of the high quality content we have published, and our authors report strong citations for their papers just in our first 9 months.

We welcome your submissions in 2016—let's do some great problem-solving this year.

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