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The future of chemical physics

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ABSTRACT

In this inaugural commentary, we offer a personal perspective which delineates past successes and future challenges of 21st century chemical physics.

In over a century of developments, the discipline of chemical physics, which evolved from physical chemistry, has had a major impact on chemistry and all related molecular sciences, including biology and materials science. While physicists were working to decipher the structure of the atom—and indeed managed to tame it—chemical physicists were trailblazing into the world of molecules with new tools, some from physics, and new concepts. In retrospect the impact is monumental, considering that in 1938 the most versatile organic laboratory instrument was the thermometer!

Today, NMR and optical spectroscopy, X-ray diffraction and electron microscopy, and LASERs and their variants are essential tools for any department actively involved in research and teaching. The "transition state"—formerly the phantom or ephemeral state—is no longer just a theoretical concept, and the nature of bonding between atoms is now well elucidated, far beyond the original description of G.N. Lewis and the theory of Heitler and London of the early 1900s. Furthermore, theoretical methods, together with the availability of high-speed computers, are enabling computations of electronic structures and trajectories of atomic motions for simple and increasingly complex systems, including biological macromolecules as well as bottom-up analysis of macroscopic material properties.

In the 20th century, chemistry was the science of molecular synthesis, structure, and dynamics, defining the principles involved in making substances, building static architectures, and observing motions of atoms during reactions. The concepts developed then have provided the foundation of molecular science: *the nature and dynamics of the chemical bond*. The methods and techniques have evolved over the years culminating, for molecules and their transformations, in the determination of complex structures, and their ensemble's behavior, and the spectroscopic observation of ephemeral chemical and biological changes, thus painting the mechanistic picture of these processes with atomic-scale resolution. The scope of applications is wide-ranging.

In part because of this success, some in the profession now think that the field in the 21st century is at "the end," perhaps only useful in service to other fields. Even more broadly, some writers of popular books have claimed the end of science! This view is shortsighted. I argue that opportunities in this century are even more exciting than, and as significant as, in the past, provided that we do not restrict our vision to orthodox boundaries and keep in perspective the core objective of chemical physics.

Chemical physics can and should remain a fundamental field of science providing new tools and defining new concepts, but with the lens being focused on significant questions in emerging areas of molecular complexity which span the gamut of applications at the frontiers of chemistry and biology. In complex systems, we still do not fully understand how hydrophobicity governs life processes (with the three-atom water matrix being an integral part of such processes), how different weak forces lead to self-assembly, how (super)phase transformation of materials occurs at the molecular level, how the forces at interfaces determine unique properties such as self-organization and spatial order, and how molecules recognize other molecules in complex environments, confined structures, or biological cells. Opportunities are numerous at

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Fig. 1. Raphael's School of Athens. Exactly five centuries ago, between 1510 and 1511, Raphael captured in his painting the intellectual discourse of philosophers most probably thinking about the fundamentals of nature. Natural philosophy, the fundamental science of today, remarkably emphasized dialogue of civilizations in the quest for knowledge, regardless of race or gender. Shown in the painting, among others, are Plato, Aristotle, Ptolemy, Hypatia of Alexandria, Pythagoras, Alexander the Great, Averroes, and Euclid (Archimedes). Note also the beauty of the place where the discourse was held, especially when compared with many of the present-day, "modern", university buildings.

the crossroads of physics and biology, or chemistry and materials science.

In a sense we are returning to Aristotelian times (see Fig. 1) when the boundaries of knowledge were less structured. Today, physicists are exploring the world of (macro)molecules and novel materials, from polymers to potentially superconducting organic and inorganic substances, and biologists are increasingly invoking the concepts of molecular bonding and the techniques of kinetics and dynamics. The increasingly important role of precision tools and quantitative descriptions of biological systems is evident in, e.g., the analysis of gene expression at the level of a single cell. Already emerging are fields at the crossroads of physics and biology through chemistry such as Physical Biology. And, the confluence of the chemical art of synthesizing semiconducting and other materials on the nanoscale with the physics of their emergent behavior, and with explorations at the cell level, is another new frontier.

Understanding processes on the vast range of length and time scales from the bottom up—from atoms to cells, or from atoms to functional materials—calls for new thinking of the evolving *nano-to-micro* structures in their nonequilibrium states, and on timescales ranging from *femtoseconds to seconds*. The function of complex networks, as in systems biology, depends critically on the degree of coherence among the different components involved, and consequently, the top-down characterization of spatial connectivity (pathways) and temporal coherence, relative to the time of the function, requires 4D visualization in both space and time. Such visualization will significantly impact a variety of areas: synthesis of functional (intelligent) materials; molecular recognition and drug design; macromolecular design and reinterpretation of the genetic code; energy, environment, and global stewardship; and functional microsystems, including MEMS and biological machines. Chemical physicists have the challenging opportunity of uncovering the nature of and the forces within the complexity of these systems and their guided functions.

Breakthroughs will continue to emerge when applications of visualization methods extend into systems of thousands of atoms and cells, and when the pertinent concepts are generalized with the help of "simple, but not too simple" theories. Computations should be considered as tools, keeping in mind that large-scale computations without a "final" theoretical condensate (or better yet, a "simple equation") are like large-scale experiments which produce numerous results that do not boil down to a meaningful finding. From both experimental and theoretical studies, the ultimate goal is to provide an understanding of the function from knowledge of structure and dynamics on different length and time scales. It would be naive to ignore the evolution of dynamics on these different scales, beginning with atomic motions, just as ignoring the "big bang" would be misleading for an understanding of the evolution of planets in the cosmic network. In the end, we may or may not find that the whole is greater than the sum of its parts, and learn why nature has designed unique, classical functions in the quantum world of atoms and molecules.

From my perspective, the discipline of chemical physics will become merely a service to other fields only if sight is lost of its primary objective; namely, to provide the fundamental concepts and the new tools that enable understanding and control of the systems behavior, from molecules to cells. The technological benefits will follow, as history has taught us, with many examples. No one would have thought that "a solution looking for a problem," the LASER, would have the technological impact it has today, from eye surgery to the information technology revolution. In Paris, we recently celebrated the 50th anniversary of the invention of the laser and Charlie Townes reminded us that it all began with an academic exploration into microwave spectroscopy of molecules, which later led to the ammonia MASER. In this Odyssey, there were fundamental issues to address, such as how to enhance Einstein's stimulated emission over absorption, how to sustain the gain, and how to achieve purity (coherence) by "beating" the uncertainty principle. It seems certain that the developments of the MASER and LASER have followed the natural course of scientific research, which was driven by intellectual curiosity!

If chemical physicists look ahead with intellectual curiosity to examine the fundamentals of nature, unswayed by fad or funding, I believe that the discipline will be here to stay. If so, in a century from now, someone else will be writing about its transformative achievements and impact, not only in science but also on society.

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