The Changing Landscape of Physical Chemistry at the Beginning of the 21st Century

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There are major changes occurring in the way research is performed in physical chemistry. This is in part due to our success in providing an ever-increasing science component to existing and emerging technologies that accelerates their need for even more. Our ability to study the science of chemical complexity permitted us to target major scientific and societal problems that require an interdisciplinary approach. These include environmental chemistry, problems of size reduction in microelectronics that led to the rise of nanoscience and nanotechnologies, and the design of drugs and implant devices that extend human life span and sustain the health of the human body.

How did this come about? Our success in devising instruments for molecular-level studies of systems in the gas phase, in condensed phases, and at surfaces produced new science. It also permitted studies of systems in ever-widening temperature and pressure ranges, with constantly improving time resolution, spatial resolution, and energy resolution. With the aim of understanding simple model systems on the molecular scale at first, the structure and dynamics of small molecules, monatomic and diatomic solids and their surfaces, were studied. These investigations then opened the door for the exploration of more complex systems such as proteins, molecular machines, and complex catalytic reactions. The remarkable progress in experiment has stimulated and has benefited from the coming-of-age of applied theoretical chemistry. It is nowadays possible for quantum chemistry to provide quantitative predictions of structure and energetics for systems of realistic chemical interest, and dynamicists and statistical mechanicians are able to use this as input for the quantitative understanding of reactivity and the formation and temporal response of molecular assemblies.

Biological or environmental systems are complex. Most technologies that produce polymers, drugs, catalysts, microelectronic circuits, or magnetic storage disks are complex. Their fabrication and development require an integrated quantitative approach involving many fields of chemistry: synthesis, characterization, and function, or physical property studies, along with applications of solid-state physics, electronics, and biology. The pursuit of nanosciences, one of the frontier fields of physical chemistry, definitely requires and benefits from this approach.

(a) The increasing science component in most technologies that drives them to become high technology, (b) our ability to tackle chemical complexity, and (c) the interdisciplinary approach necessary for success in producing new science in many fronts of physical chemistry are all causing us to rethink the way research is performed in the field. The use of single instruments to perform measurements and the compartmentalization of synthesis, characterization, and studies of properties no longer fit the purpose which is to solve major science or technology problems. The division of physical chemists to groups that investigate molecular behavior in the gas phase or in the condensed phase is no longer possible, as most problems that involve physical chemistry have both gas-phase and condensed-phase components. Interfaces are where much of the current interest is, whether the coupling of a molecule to an electrode or the biocompatibility of implant devices and molecular recognition in general. The increasing human power cost of research, which rises more rapidly than the costs of instruments, requires that each investigator be knowledgeable in the use of several instruments. The same researcher should be able to carry out characterization and property studies requiring a broader and more interdisciplinary education. When short pulse lasers can be used at the diffraction limit, we would need all the integration that is humanly possible.

Physical chemistry has gone through one period of integration followed by a period of decentralization before. In the beginning of the 20th century, the rise of quantitative analytical techniques, thermodynamics, and macroscopic kinetics spawned chemical technologies ranging from ammonia and methanol synthesis to the internal combustion engine. The rise of quantum mechanics opened the door for studies of molecular structure and bonding and led to the development of many instruments for spectroscopic studies of gas-phase molecules and diffraction studies in the condensed phase. Decentralization and specialization have served us well to reach a molecular understanding of many simple chemical systems. By the 1950s, this knowledge permitted the studies of complex molecules. Pauling published the structure of topaz determined by X-ray diffraction in 1928. In 1951, his eight publications in a single issue of PNAS established the helical structure of proteins, a great increase in the complexity of chemistry that could be tackled on the molecular level. The increasing complexity of systems that can be explored is also evident from NMR studies, as shown by recent Nobel Prizes. The continuous push for improved time, spatial, and energy resolutions opened up new domains of physical chemistry research. From the 1950s, the discovery of the transistor provided the thrust for molecular surface chemistry, because this and other technologies developed in subsequent years improved by size reduction—the smaller they are the more efficient they become. The techniques of modern surface chemistry permit the atomic level studies of $10^{13}-10^{15}$ atoms per cm^2 at the surface in the background of 10^{22} per cm^3 in the condensed phase. The simple, single-component model surface systems that were studied at first are being substituted by more complex surfaces, polymers, biopolymers, electrodes, and multicomponent catalysts as our molecular-level understanding improves.

Now enter the nanosciences, which again are also driven by the needs of technologies, which provide challenges to learn the manipulation of matter on the nanoscale: connecting molecules and studying their self-assembly, optical, chemical, electronic, magnetic, and mechanical properties. The centralizing themes of physical chemistry again become dominant at the start of the 21st century, just as they were dominant in the early decades of the 20th century.

Up to the later 20th century, our thinking in physical chemistry was conditioned by the concept of a fairly rigid molecular structure. When we allowed displacements from

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equilibrium, they were taken to be small enough that there was a restoring force bringing the system back. The barriers to isomerization or to reaction were taken to be larger than kT. When reaction did take place, the potential-energy landscape was assumed to be simple enough that there was a clear reaction path leading to the products. Unusual cases such as the van der Waals molecules or clusters were exceptions to the norm. But the complex systems of current concern force us to recognize fluxionality as the norm. There are numerous energetically low-lying isomers so that weak interactions, many of which can be thought of in mechanical terms, are essential for the action of the system.

There are more technology challenges to come! Energy conversion and storage require learning how to produce hydrogen, the development of fuel cells, and learning how to sequester CO_2 and mine methane hydrates in the continental shelf and convert them to liquid fuels. The development of polymers as structural materials and of biopolymers that are biocompatible with the human body is within our reach. The encapsulation of nuclear waste in a way that lasts for centuries using glasses, ceramics, and composites is a major challenge. The development of defense science that uses sensors and remote sensors to improve personal safety and the exploration of outer space all require new science and an interdisciplinary approach to tackle the chemical complexity that is involved. Catalysts must have 100% selectivity for desired reactions to eliminate byproducts (waste). Green chemistry requires an understanding of the molecular ingredients that control selectivity. Enzymes do exhibit this kind of selectivity, and synthetic catalysts must be able to attain their level of selectivity.

Physical chemistry is a vibrant ever-changing central field of science. The push of high technology, nanosciences, increasing labor costs, and the need to understand biological complexity and many other complex systems on the molecular level drive the integration of disciplines at present—and we suspect for many years to come.