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Historical Developments in Physical Chemistry

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Letter to the Editor

Since the first introduction of the term "physical chemistry" by Mikhail Lomonosov in 1752 during his lecture on a new science [1] entitled "A Course in True Physical Chemistry" before the students of Petersburg University, the field of physical chemistry has produced a continuous stream of conceptual advances, methodological innovations, and new applications that continues to the present day [2-6]. For those who are not active researchers in the field of physical chemistry, it is worthwhile to list some of the milestones in its history, which include:

1. The publication of the article in 1876 entitled "On the Equilibrium of Heterogeneous Substances" by Josiah Gibbs which set the stage for the Gibbs energy and chemical potentials as well as numerous analogs in Gibbs' phase rule [7,8];
2. The enthalpy that is measurement of energy in a thermodynamic system and is the preferred expression of system energy changes in many chemical, biological, and physical measurements at constant pressure, because it simplifies the description of energy transfer;
3. The leading figures in physical chemistry in the late 19th century and early 20th Century were Wilhelm Ostwald, Jacobus van't Hoff, and Svante Arrhenius who created in 1887, the first scientific journal in the field of physical chemistry, Zeitschrft fur Physikalische Chemie (Journal of Physical Chemistry);
4. The application of statistical mechanics to chemical systems and work on colloids and surface chemistry where Irving Langmuir made seminal contributions in early 20th Century [9];
5. The important step forward was the development of quantum chemistry in the 1930s, where Linus Pauling was one of the leading names who made tremendous contributions in the field of physical chemistry;

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6. The quantum chemistry involvement in the interchange of experimental and theoretical techniques, where the use of different forms of spectroscopy, such as infra-red spectroscopy by Sir Frederick William Herschel in 1800, microwave spectroscopy by James Clerk Maxwell in 1864, nuclear magnetic resonance by Edward Mills Purcell and Felix Bloch in 1940s, electron paramagnetic resonance by Yevgeny and Zavoisky in 1944, and scanning tunneling microscopy spectroscopy by Gerd Binnig and Heinrich Rohrer in 1981, is doubtless the most foremost development in the last three centuries;
7. The recent discoveries in astrochemistry with the deeper understanding of isotopic fractionation, especially involving deuterium during star formation, and a realization that the role of neutral–neutral reactions is more salient than once thought possible [10];
8. The development of the calculation of algorithms in the field of additive physicochemical properties that has transformed contemporary physical chemistry. As a result of these and numerous other developments, physical chemistry is now a central field in nearly all areas of the physical and chemical sciences.

Physical chemistry, in contrast to chemical physics, is predominantly a macroscopic science, focusing mainly on macroscopic properties of an ensemble as the majority of the physical laws on which it was founded relate to the bulk rather than the molecular or atomic structure alone. Chemical physics on the contrary, studies chemical ensembles and reactions from a physicist's point of view and sometimes it is also treated as a subfield of physical chemistry [6]. In modern times the various fields are not separated by a sharp line and they most likely overlap into each other. Yet, given the apparent simplicity in the preamble of Mikhail Lomonosov' lectures ("Physical chemistry is the science that must explain under provisions of physical experiments the reason for what is happening in complex bodies through chemical operations"), a naïve scientist might wonder how physical chemistry can remain a vibrant field of research after more than 260 years of contributions from brilliant scientists. Certainly, the spectroscopy techniques available for physical chemistry experiments have increased significantly in every century since Isaac Newton (the development of spectroscopy is inextricably linked with advances in the theory of light, refraction, and diffraction that began in the mid-17th century), and the speed and capacities of digital electronics, computers, and storage media in modern times have improved dramatically [2]. These spectroscopy methods and other technological advances are important aspects of progress in physical chemistry, but, by themselves, they might be expected to produce only quantitative improvements in physical chemistry data rather than qualitative breakthroughs. So how can qualitative breakthroughs in physical chemistry methods and applications continue to occur? There are several answers to that question. One at least is that physical chemistry problems in modern sciences rely mainly on molecular structure, quantum chemistry, and general theory. Spectroscopic methods are used to determine the nuclear positions in a molecule. Theoretically, the molecular structure is determined by solving the Schrodinger equation for the motion of the electrons in the field of the nuclei and the determination of structures by numerical solution of the Schrödinger equation has become a highly developed process entailing the use of computers and supercomputers [11]. Major goals of quantum chemistry include increasing the accuracy of the results for small molecular systems and also increasing the size of large molecules that can be processed which is limited by scaling considerations [11]. This methodology creates the possibility of manipulating electrons and atoms evolution in an endless variety of ways, which can be accurately described by wave model, valence bond, molecular orbital and density functional theory that lend themselves to creativity and new insights.

This short letter describes advances in physical chemistry and spectroscopy over the time. I hope this letter will help bring the current vitality of physical chemistry research to the attention of the broader chemistry and physics community and lead to new interactions between physical chemist specialists and specialists in other fields. I thank the leading authors for their contributions. I also thank the Editors of Physical Chemistry: An Indian Journal for honoring me with the invitation to publish this short letter.

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