Brochure Physical Chemistry (SFC)

This brochure has been put together by a number of European physical chemical societies or divisions in order to describe the profile and the role of the physical chemist. It primarily addresses students who are interested in learning more about a career in physical chemistry, but it may also be helpful to technologists and science administrators.

* one section per country, plus information at the European level where appropriate

1. Introduction

Physical chemistry aims at understanding the structure, properties and transformations of matter, from bulk behaviour down to mechanisms at he molecular level. It is the role of the physical chemist to collect, collate and analyse experimental data from all branches of chemistry and to construct predictive models. As such, physical chemistry underlies much of modern science and is a motor driving advances in a very wide range of fields. Building on information and concepts from chemistry, physics and mathematics, physical chemistry contributes to and is stimulated by areas as diverse as medicine, molecular biology, biochemistry, molecular engineering, chemical engineering, materials science and earth sciences.

This brochure begins with a brief historical introduction, the main areas of physical chemistry are then described, the most important challenges are highlighted and the impact on society as a whole is considered. The career of a physical chemist in research, education, industry is then discussed. The professional societies are presented and, finally, a list of sources of information concerning physical chemistry is provided.

2. A brief history

Physical chemistry has an illustrious history stretching back almost 300 years and, until the 20th century, it has largely been a European enterprise. Throughout this period, physical chemists have played major roles in the development of modern physical sciences and have had far reaching impacts on industry and society. Studies of the physical aspects of chemical systems began in the18th century with great scientists such as Lavoiser, Davy, Berzelius and Lomonosov who laid the foundations of modern chemistry, simplified chemical nomenclature and began investigations into such important processes as combustion, catalysis, corrosion, analytical chemistry and reaction kinetics. From this period onwards, strong interactions were formed with mathematics, physics and the developing science of living systems, where one can cite the work of Lavoisier on the chemistry underlying animal respiration and of Galvani on the role of electricity in living systems, which the contributions of Volta, led to the development of electrolysis.

The passage to the 19th century saw much interest in the behaviour of gases and ionic solutions, which laid the pathway to the development of the atomic theory (Dalton, Avogadro, Gay-Lussac) and the importance of molecular interactions (van der Waals), ideas upon which much of modern science has been built. This step was vital to the evolution of concepts such as stereochemistry (van’t Hoff, Berthelot), isomerism (von Liebig, and Bunsen, who also developed chemical spectroscopy and made the first step in photochemistry) and indirectly led to the end of the doctrine of vitalism (berthelot). At he same period, great strides were also made by Faraday, who notably established the field of electrochemistry. This century also saw the foundation of chemical thermodynamics, chemical kinetics and statistical mechanics (Gibbs, Le Chatelier, Oswald, Nerst) which played no small role in the explosive growth of chemical industry during this period.

This rapid progress accelerated still further with the arrival of the 20th century and, notably, the discovery of natural (Becquèrel, Curie) and artificial radioactivity (Joliot-Curie). This period also saw a deepening, of our physical understanding of atomic structure which, through the development of quantum mechanics, led to theoretical and practical developments in valence theory (Lewis, Pauling, Onsager, Coulson) and radiochemistry (Soddy, Urey). Many major physical techniques were also developed during this time, amongst which one can cite electrophoresis and chromatography (Tizelius), ultracentrifugation (Svedberg), mass spectroscopy (Aston) and the use of molecular beams (Stern). This century has also seen progress in understanding the statistical mechanics and thermodynamics of non-equilibrium systems (Hinshelwood, Prigogine), the behaviour of complex systems and polymers (Flory, de Gennes) and notable developments in spectroscopy (Porter, Ernst) and the theory of chemical reactivity (Marcus).

3. Physical chemistry today

Today, the classical aspects of physical chemistry, thermodynamics, kinetics and reactivity are being developed in numerous active areas such as spectroscopy, photochemistry, polymer science, electrochemistry, radiochemistry, catalysis, analytical chemistry and theoretical chemistry.

The objects studied by the physical chemist have evolved from the classical states of matter, cases, liquids and solids, to such complex systems as liquid crystals, colloids, micelles, gels, solgels and areosols. Much work also concerns the interactions which occur at surfaces and interfaces and cover the important phenomena of adhesion, wetting, friction and catalysis. The constituent elements to be studied have thus also evolved from simple atoms and molecules to organised molecular and macromolecular systems structured by weak molecular forces. Major applications comprise the creation of new materials with more sophisticated and controlled macroscopic properties including smart gels and alloys, ceramics and composites, superconductors and ferrofluids. One should also cite the exciting new nanoscale structures which include fullerenes and nanotubes.

Structural investigations of these objects are profiting from many advances in traditional techniques such as X-ray diffraction, where low angle scattering is helping to elucidate the nature of organised molecular systems and high intensity synchrotron radiation is opening the route for studies of microcrystals and of time-resolved conformational changes. Similarly, high field strength and multi-dimensional analysis are extending the applicability of NMR spectroscopy, which, today, also plays a major role as a medical imaging tool. Neutron scattering has become as well a powerful technique to gather information on both structure and dynamics. At the finest level, new microscopes (STM: scanning tunneling microscope; AFM: atomic force mcroscope) are probing down to individual atoms and molecules, and revealing, for example, the astonishing complexity of surfaces once thought of as regular objects. Beyond observation, it is even becoming possible to manipulate both individual atoms and molecules in order to study their mechanical properties and their interactions.

In terms of time, the limits of observation have been pushed to the femtosecond scale, enabling, the study of extremely short-lived species and phenomena such as coherent effects and ultrafast energy and charge transfer. Other limits targeted involve chemical reactions under extreme conditions of pressure or temperature, with many applications ranging from the study of plasmas or the chemistry of interstellar space to crystallisation under conditions of microgravity.
Many links have been established with structural and molecular biology, enabling a deeper understanding of the organisation and interactions of biological macromolecules and the fundamental aspects of biological metabolism. Physical chemistry is helping, to analyse the mechanisms of molecular recognition, in molecular machines as complex as those involved in the processes of gene transcription, cell division and cell mobility. In return, better knowledge of living systems is leading to the development of biomimetic materials and new molecular probes and sensors. In addition, the sophistication and selectivity of enzymes and antibodies are being put to use in many chemical applications. Medical techniques such as phototherapy and drug targeting are also profiting from the know-how developed by physical chemists.

As physical chemistry moves forward the systems studied become more complex and there is an increasing need for reliable and predictive computer simulation which helps to interpret and orient experimental research. In this area simulations are progressing towards a refined quantum mechanical description of the interactions, excitations and reactions of small molecules and also towards more realistic descriptions of the structure, stability and dynamics of macromolecular systems and molecular assemblies, taking into account the effects of complex solvent and ionic environments.

4. Impact on an evolving society

Physical chemistry impinges on many factors which will determine the quality of our lives in the future. Firstly, one can cite the need to find new and more efficient means of energy production and ways to conserve and to recycle non-renewable resources. In this area, much remains to be done to improve batteries, fuel cells and solar cells. Secondly, it is necessary to develop clean industrial processes and to solve the multiple problems involving pollution, toxic chemicals and radioactive waste. This equally implies developments in detection, treatment and mechanistic analysis, which are all areas where the physical chemist makes a major contribution. Thirdly, important strides can be made in agricolture and medicine through a better understanding of the underlying physico-chemical processes. Lastly, through fields such as art or architectural preservation, physical chemistry contributes to our cultural heritage.

5. The career of the physical chemist *

In France, university studies in physical chemistry begin after the Baccalauréat with a two year DEUG diploma (Dipl6me d'Etudes Universitaires Générales). Most students chose the option dealing with the science of matter which provides a general culture in physics, chemistry, mathematics and computer science. The next step, which involves more specialisation, are the "Licence et Maitrise de Chimie Physique". These courses deal with both theoretical and experimental aspects of physical chemistry and require two years. Students wishing, to study for a doctoral thesis, must then undergo a final year of specialisation, obtaining a DEA (Diplóme d'Etudes Approfondies) in a defined field of physical chemistry. This involves roughly six months of courses and a six month research project. An alternative route involves the "Grandes Ecoles" which offer their own degree courses. In particular, one can cite the Ecole Supérleure de Physique et Chimie Industrielle, based in Paris. Doctoral studies require three years of work. The thesis prepared by the student should contain original results and demonstrate his or her ability to carry out research. Students wishing to look for a job more quickly can follow an alternative route and take a more applied DESS (Diplòme d'Etudes Supérieurs Spécialisées) course which lasts one year.
Substantial grants are available for students doing doctoral theses. These come principally from the Ministry of Education and Research, but can also by financed partially or wholly by industry or by other organisations.
European “Marie Curie” grants are also available for students undertaking research outside their native country.
Small grants are also available for most DEA students.

Following these studies, a number of career choices are open to the young physical chemist:

Physical chemists are involved in teaching at many levels, ranging from colleges to Universities and engineering schools (“Grandes Ecoles”). Typical qualifications needed for college teaching are obtained after one year of studies by national competition and include the “CAPES” and the “Agrégation”, while university posts generally require a thesis.

Academic research in France involves both university staff, staff in the engineering schools (“Grands Ecole”) and many research scientists employed by the national research organisations. The largest of these bodies is the CNRS (Centre National de la Recherche Scientifique), but physical chemists also belong to the CEA (Commisariat à l’Energie Atomique) and, more rarely, to the medical or agronomie organisations, INSERM (Institut National de la Santè et de la Recherche Méedicale) and INRA (Institut National de la Recherche Agronomique). All the research organisations also offer engineering and technical posts. Scientists are typically recruited after completing their doctorates and one or more years of post-doctoral studies and competition is naturally high.

Physical chemists work in French industries dealing with, for example, chemicals (Atochem), cosmetics (L’Orèal), food production (Danone), pharmacology (Rhone Poulenc Rorer), petrochemicals Elf Aquitanine), glass and ceramics (Saint Gobain), electronics (Thomson). Physical chemists play important roles in transferring processes from the laboratory to industrial production, process design and optimisation, as well as safety and quality control. Extraction, purification, mixing, formulation and combustion processes are all aspects of this task. Production management, developments in instrumentation and technology transfers are also handled by the physical chemist.

Amongst other important areas involving physical chemists it is worth citing increasing sophisticated forensic science and the study, restoration and preservation of works of art. However, a career in physical chemistry may also lead to the broader fields of finance, marketing, patenting and management. With the development of the European community many new openings are appearing in the areas of norms (AFNOR, European Normalisation Committee), standards and regulations. Qualified specialists are also required for the definition of safety procedures and the classification of toxicological risks. Beyond these technical areas, physical chemists can also put their knowledge to good use in diffusing scientific information to both general and technical audiences and in dealing with the major legal and ethical questions raised by modern scientific research.