Challenges and Opportunities of Chemical Sciences In The 21st Century

Rina Saha

Department of Chemistry, Govt. Maharani Sudarshan College, Bikaner, Rajasthan.

Abstract

The article will identify the recent advances and current challenges in fundamental understanding of the basic science, and it will explore the impact beyond the chemical sciences that these advances have had in the past. It will also explore the possibilities for such impact in the future, recognizing that such developments are frequently serendipitous. A key goal of the chemical sciences is the creation of molecules and materials that do not exist in nature. The ability to design and synthesize new substance offers the possibility of improvement on what is found in nature – with both accomplishments and future opportunities that range from life saving drugs to material that can help to make our lives safer and more pleasant. Chemistry has a key role to play in the area of analysis and structure determination which presents important and exciting needs, opportunities and challenges such as. detecting toxic or explosive materials in the environment detecting land mines and making chemical manufacturing processes environment friendly via real time control. Thus the Chemical Sciences have not only a great past but an even more exciting future.

Keywords: synthesis, transformation, green chemistry, computational chemistry.

Introduction

Chemical Science is involved in everything, it is the basis of life, and without it we would not exist. This article gives an insight to the research, discovery and invention across the entire spectrum of activities in the chemical sciences – from fundamental molecular level chemistry to large scale chemical processing technology. The drive towards clean technology in the chemical industry (green chemistry) is providing challenges to the chemists, educationists and researchers. With these challenges, there are an equal number of opportunities to discover and develop new products, processes and services that achieve the societal, economic and environmental benefits that are required. The interaction between fundamental research and application is not a linear, unidirectional one in which basic ideas are spawned in isolation and flow inexorably an important application. A more realistic representation of the interaction applicable to the chemical sciences is the quadrant model of Stokes.[1] The main point of the quadrant model is that just as fundamental science is not always aimed at producing technology, neither does science always precede technology. It will be necessary for scientists to produce major new discoveries, revolutionary new technologies and important new additions to the quality of life for our society. They must also stand ready to play a major role in assisting the government and shaping its policies to benefit all our population. The history of science repeatedly shows that major discoveries open up whole new areas of understanding and of practical applications that were not anticipated.

Synthesis & Manufacturing

Chemist wants to understand not only the substances and transformations that occur in the natural world, but also those that are permitted by natural laws. Thus the field involves both discovery and creation. They want to discover the components of the chemical universe – from atoms and molecules to organized chemical systems such as materials, devices, living cells, and whole organisms and want to understand how these components interact and change as a function of time. They also consider the unknown molecules & substances and interactions that could exist. Science has become increasingly interdisciplinary. Investigating a single compound, a single reaction or a single process may fall within the expertise of a single discipline or subdiscipline but the situation is different when the investigations are extended to systems – full assemblages of related components that address the same function or to processes, where integrated systems of operations work in concert to produce a product. Understanding, developing, manipulating the systems and processes often require the synergistic advantages of the entire range of the chemical sciences – from fundamental chemistry, to chemical engineering, and advanced areas of science and technology, to create scientific understanding and benefit for society.

The goal of the basic science is to invent new types of transformations. Transformations are part of the universe of chemistry and they are the tools that make possible to create interesting and useful new substances. It is also important to invent overall strategies to achieve multistep syntheses involving a sequence of transformations. In synthesis and chemical manufacturing there is a general need to develop separation methods. There are two goals related to separations. One is to learn how to isolate and purify the desired components with high efficiency, and the other is to develop synthetic processes that do not need such separation.

For manufacturing, a further goal is to eliminate solvents or at least replace them with harmless inexpensive and easily removed or recovered solvents. The extra chemicals produced during chemical reactions must be removed and disposing of them adds cost and the potential for environmental problems.

A synthetic chemist after recognizing the challenge looks for inspiration in several places for transformation that cannot be done with current methods. Synthetic inspiration can come from an attempt to make drastic improvements in the properties of existing substances. For example, some metals and metal compounds become superconducting at extremely low temperatures.

Challenges and Opportunities for the future

In spite of the impressive progress achieved by synthetic chemists in the past several decades, the state of the art of methods for chemical synthesis remains at an early stage of development. There is great need for new reactions and synthetic methods to permit any substance, of any complexity, be it organic or inorganic in structure, to be synthesized with high chemical efficiency, in a small number of steps and with minimal cogeneration of any waste products.

Synthesis and manufacture is important because the expansion of chemical universe through synthesis leads to great new scientific insights. The promise of better medicines and better materials depends on the ability of synthetic chemists to create new transformations and to use them in the creation and manufacture of new substances.

Chemical and Physical Transformations of Matter

A principal goal of the chemical sciences is to understand and manipulate chemical and physical transformations of matter. Transformation means a change in composition, state, or organization of matter, or movement or rearrangement of materials by flow, heat or diffusion. A chemical transformation can occur when molecules collide with sufficient energy. Generally a reaction occurs when the molecules are heated or irradiated to provide the energy necessary to overcome the activation barrier that separates reactants from products.

The detailed molecular structures involved throughout the entire procession from starting materials through the transition states to products in a chemical reaction are so far no directly observable, there are certain classical ways in which reaction mechanisms are effectively deduced. One route is through the use of kinetics, the observation of how the rate of a reaction depends on concentrations of various components, and on temperature and sometimes pressure.

Some chemical reactions, such as the change of diamond to graphite under normal conditions of temperature and pressure or the spontaneous conversion of left-handed to right-handed amino acids, are so slow that their rate of change is measured in millions of human lifetimes or longer whereas the photodissociation process is so fast that typically takes 10 to 100 femtoseconds. Thus Chemical scientists possess the tools to make kinetic measurements over the full range of reaction rates.

Super critical fluid processing is exploiting knowledge about this domain of phase behaviour for new applications in separations, chemical reactions and materials production. Supercritical carbon- dioxide is now used as a solvent in improved, environmentally benign methods for decaffeination of coffee and for dry cleaning.

The importance of physical transformations in making chemical products implies a vast opportunity for understanding structures of many kinds of important chemical products at higher levels and longer length-scales than those of individual molecules.

Chemists have synthesized a spectacular array of submicron – and nano particles with well-defined size and atomic structure and very special properties.

Transport phenomena play crucial roles in both the creation and performance of structural chemical products. It presents an important challenge in the progression toward smaller length-scales of microscale, nanoscale and molecular scale. Chemical processing will need to exploit small-scale reactors in new applications.

Challenges and Opportunities for the future

The femtosecond spectroscopy has made it possible to observe reactions on a short time scale, a major challenge is to devise ultrafast techniques that will permit observation of the actual molecular structure of a transition state, not just its rate of passage. As a general goal, we want to be able to make moving pictures of the reactions themselves, observing all the intermediate states and the rates at which they interconvert. Such moving pictures can be generated even now, by computer simulation of the reaction: the problem is to determine whether those pictures are correct. Thus a second challenge is to interface with theoretical chemistry in getting the best possible calculations, and then devise experimental tests of the major theoretical predictions to see whether experiments confirm the correctness of the calculations.

Much work has been done to understand how metal ions react or catalyze the reactions in solution. There is still need to understand how the enzymes work. When we do understand them in detail, we should be able to produce biomimetic catalysts for useful processes in manufacturing.

Isolating, Identifying and Measuring substances

Chemical scientists want to explore the natural world and identify all its chemical components. They also want and need to identify all the new chemical substances produced directly and indirectly as a result of their synthetic and manufacturing endeavors.

Detecting known substances and determining their quantity is also important. In synthetic research, it is essential to know the relative proportions of various reaction products. In manufacturing it is important to detect any impurities in the product and to determine whether they are present in a significant amount.

The frontiers in this field lie in improving sensitivity to detect vanishingly small quantities, to separate extremely complex mixtures of chemical substances and to assess the structures or compositions of components. Measurements using very small or very dilute samples can present a major challenge in clinical medicine or environmental analyses. A vital activity of the chemical sciences is the determination of structure. Some molecules exist in more than one structure (conformation). Some molecules are so floppy that structural characterizations really refer to averages among several structures. Yet other molecules are sufficiently rigid that molecular structure can be quite precisely determined. The techniques available to achieve molecular structure determinations are limited eg. X-ray diffraction technique, microwave spectroscopy, nuclear magnetic resonance spectroscopy etc.

A major limitation of diffraction techniques has been the need to obtain crystalline samples. If scientists could learn how to crystallize large molecules in a routine manner, a breakthrough would result.

The “weighing” of a molecule of a chemical substance and of its fragments has great utility in both assessing molecular identity and determining molecular structure. Mass spectrometry requires that the material being studied be converted into a vapour. The invention of new ways to volatize molecules, from solids and from surfaces, has revolutionized and re-invigorated this field.

Challenges and Opportunities for the future

Chemical measurements will continue to be challenged by the broad advances of the chemical sciences. New fundamental knowledge is essential for advancement in the measurement sciences particularly in nanoscale science and technology, which are at the heart of future advances in automated storage and retrieval of information.

Chemical Theory and Computer Modeling

Computational chemistry and process systems engineering play a major role in providing new understanding & development of computational procedures for the simulation, design & operation of systems ranging from atoms and molecules to industrial-scale processes.

Science proceeds by both experiment & theory. Simple experimental facts without a theory to interpret them do not satisfy our need for understanding. Theory validated by experiment runs through all of chemistry and almost all its branches now use computers. Structures are determined by computer treatments of x-ray data, potential new drugs are analyzed by computer modeling and even synthetic strategies to make a desired target molecule are developed using computer programs created for the purpose.

Modeling and simulation are extremely important tools in the chemical sciences. The understanding of complex chemical processes depends on modeling and computation. Recent advances in computing not only have enabled more accurate & reliable calculations, but they have also provided new tools for interpreting the output of the calculations. Modern computer graphics i.e. molecular graphics, simulations and animations have greatly enhanced the ability of scientists to understand & utilize the results of their computations.

Challenges and Opportunities for the future

Improvements in DFT functionals will improve the accuracy of DFT calculations. One specific challenge will be to derive density functional theory from fundamental theory in a way that reveals how to incorporate successive approximations for the exchange & correlation terms. Some work on high level methods with better scaling may allow more immediate extension of high accuracy calculation to larger systems. We need to develop new & powerful computational methods that span from the atomic and molecular level to the chemical process & chemical enterprise level in order to allow their effective integration for multiscale simulation and optimization.

Interface with Biology and Medicine

The goal of fundamental science at the interface of chemical sciences & biology is to understand life in chemical terms. The mechanisms of life are revealed when we understand their molecular details. Moreover, molecular understanding of biology plays the major role in guiding drug discovery & molecular level understanding of biology is fundamental in developing diagnostic methods.

Molecular analysis of living cells has led to a flow plan of information in molecular biology, known as the Central Dogma: The information necessary for a cell is encoded in the double helix of DNA. Many of the computational techniques are related to recent advances in sequencing of DNA. Bioinformatics includes computational chemistry with the goals of predicting function and three dimensional shape directly from the amino acid sequence-by comparison with sequence, function and structural information for other proteins. Knowing protein structure can provide direct benefits to human health. The three dimensional structural information derived from the X-ray crystal structure combined with computer modeling techniques allowed chemists to design potent, selective inhibitors of the protease enzyme.

Challenges and Opportunities for the future

The challenge is to discover the chemical identity of all the molecules that make up living organisms and the way they bind to each other and organize into biological structure such as nuclei, ribosome etc. Our driver for new discovery will be the completion of the human genome project.

This project will help in determining the locations and sequences associated with the genes of the human genome. New and improved drugs will be required to fight disease and improve quality of life.

Materials by Design

A material is defined as the substance or substances out of which a thing is made or composed. The overall goal of materials research within the chemical sciences is to explore, design and control through synthesis and processing the relationships among structure, properties, composition that determine the useful behavior of all materials. A frontier challenge is to investigate the chemistry and properties of single isolated molecules and compare that behavior with the average molecular behavior in an assembly, solution or condensed phase of molecules. The traditionally made stable materials will last a long time and do not requires to be replaced. This longevity has the undesirable consequences of creating waste that requires significant energy to process or it clutters the landscape when discarded.

Challenges and Opportunities for the future

The science of materials reflects the way that chemistry has changed from a field concerned with atoms and molecules and their properties in isolation to a field concerned with organized interactive systems. This change opens opportunities and challenges in fundamental science to know the chemical components of the stuff and how do these components interact to produce the properties of the stuff. The solution of these questions will greatly add to understand the chemical universe.

Atmospheric and Environmental Chemistry

Geochemists have made progress in learning the chemistry of earth and its components including rivers, lakes and oceans. A field called earth systems engineering is emerging and this field will deal with global warming, carbon sequestration and environmentally benign manufacturing. It will also address new analytical, computational and assessment techniques through which global scale interaction in complex systems can be better understood and optimized.

The design, development and implementation of chemical processes and products to reduce or eliminate substances hazardous to human health and the environment is known as Green chemistry.[2] This definition has been expanded to twelve principles.[3]

To illustrate challenges and opportunities for green chemistry a simple acid catalysed reaction can be considered where Bronsted acids or Lewis acids are used. These reactions are common in chemical, petrochemical, pharmaceutical allied industries. These acids are cheap, readily available and very active but they are difficult to separate from the organic products and their use leads large volumes of hazardous waste. In the petrochemical industries the reactions are common with solid acids.[4] Solid acids including zeolites results relative low quantity of waste and can be removed from the products. The use of zeolites,[5,6] clays mixed metal oxides, functionalized polymers and supported reagents[7,8] as well as lanthanide triflates[9] for liquid phase organic reactions and ionic liquids[10] for some reactions stands solution for the problems in green chemistry.

Challenges and Opportunities for the future

Knowledge of complex chemistry by which the atmosphere and the earth react including the dependence of global climate on carbondioxide concentrations in the atmosphere is required. Scientist will need to investigate effective ways to trap or reduce the generation of carbondioxide that would otherwise build up in the atmosphere.

The consequences of human action on the environment are not always foreseeable so to meet this challenge it is essential that we continue to cultivate a strong base of fundamental knowledge in the chemical and biological sciences and tools should be prepared not only to create new technologies but also to anticipate their consequences.

Energy for Future

Scientists should invent new ways to generate and transport energy for human use and provide for the needs and aspirations of a growing population in a sustainable manner. New ways should be discovered to minimize the energy used for human activities including manufacturing.

Challenges and Opportunities for the future

The challenges and opportunities in the field of energy are critical for a world in which inexpensive, readily available fossil fuels will eventually be exhausted. We need to devise better ways to use solar energy eg. By creating cells for conversion of sunlight to electricity, replacing combustion by fuel cell technology. We need to invent rechargeable batteries that are practical for vehicles that have electric motors instead of gasoline engines.

National and Personal Security

Chemical science and technology must contribute to the enhancement of national and personal security by providing fundamental understanding and new developments to defend against military, terrorist or criminal attack and give warning of accidental or natural disasters. The goal to which scientist can contribute begin with early detection and prevention of an attack or event but if prevention is not possible, they extend to mitigation of the effects and subsequent remediation of damage. Biological warfare agents present a threat because the original viruses or bacteria can multiply and infect additional people. New vaccines and new approaches for delivering drugs and vaccines are required to discover. The development of new vaccines will need to be carried out in full recognition that genetically modified pathogens could be used in an enemy attack.

Chemical warfare agents are extremely toxic and very fast acting. Scientists must develop better understanding of their mechanism of action and use this information to device possible remedies .Research by scientists will be required for the development of new analytical techniques to detect nuclear proliferation threats and treaty violations. This will require establishing the characteristic signatures of both production and testing of weapons. Detection of these signatures will depend on chemical spectroscopy techniques and advances in remote sensing.

Conclusion

The scope of the chemical sciences endeavor is vast, contributing far beyond the tradition aspects of chemistry. As a consequence, opportunities for fundamental and creative science and major contributions to technology and society will remain in the hands of chemical scientists for a long time. New fundamental chemical insights will increase our scientific understanding and the practical importance of future discoveries will have enormous potential.

The solutions to all these challenges can be achieved by the research work done by the chemists in collaboration with scientists from different disciplines. The scientists need to communicate effectively to the general public through the media as well as directly to convey the goals and achievements of chemical sciences in pursuit of better world. The help of young bright students should be taken to meet these challenges. They can contribute to critical human needs while following exciting careers, working on and beyond the molecular frontier.

References

1. Donald E. Stokes, Pasteur's Quadrant, 1997, Brookings Institution Press, Washington D. C.

2. P. T. Anastas and J. Warner, *Green Chemistry Theory and Practice,* 1998, Oxford Science, Oxford.

3. M. Poliakoff, J. M. Fizpatrick, T.R. Farren and P. T. Anastas, *Science*, **297**, 807-810, 2002.

4. J. M. Thomas and W. J. Thomas, *Heterogeneous Catalysis*, 1997, VCH, Weinheim

5. T. Bastock and J. H. Clark, *Speciality Chemicals*, 1992, ed. B.Pearson, Elsevier, London,

6. S. Ratton, *Chim. Oggi*, 33, 1998.

7. J. H. Clark, *Catalysis of Organic Reactions by Supported Inorganic Reagents,* 1994, VCH, New York,

8. J. H. Clark and D. J. Macquarrie, *Chem. Commun.*, 853, 1998.

9. A. Kawada, S. Mitamura and S. Kobayashi, *J. Chem. Soc.,Chem. Commun.*, 1157, 1993.

10. C. J. Adams, M. J. Earle, G. Roberts and K. R. Seddon, *Chem. Commun.*, 2097, 1998.