Pure & Appl. Chem., Vol. 69, No. 2, pp. 255–256, 1997.
Printed in Great Britain.

The physical organic chemist as a materials scientist in the 21st century

Meir Lahav

Department of Materials and Interfaces, The Weizmann Institute of Science, Rehovot, Israel

Biography: Meir Lahav studied at the Hebrew University of Jerusalem, and received the M.Sc. in 1963 in the field of organic polymers, and the Ph.D. in 1967 for studies of organic solid state reactions. After postdoctoral work with P.D. Bartlett at Harvard he joined the Weizmann Institute of Science in 1971, where he is currently Head of the Department of Materials and Interfaces, and Director of The Minerva G.M.J. Schmidt Interdisciplinary Center of Supramolecular Architectures. He is incumbent of the M. Thatcher chair of chemistry. He has been the recipient of the Kolthoff Prize of Chemistry from the Technion in Haifa and the Prelog Medal for Stereochemistry (with L. Leiserowitz) from the E.T.H. in Zurich, and was Centenary Lecturer of the Royal Society of Chemistry. He has research interests in the origin of chirality, stereochemistry, mechanistic study of solid state reactions, crystal engineering, thin organic films, and related fields.

Looking at the future is a dangerous and often futile exercise. Discoveries are generally hard to predict and therefore one can only try and delineate areas of future developments. The physical organic chemist has developed over the years methodologies which provide deep and detailed knowledge of the various reaction pathways taking place in the breaking and making of chemical bonds, and in the structural stereochemistry of organic compounds. In recent years these methods have been successfully extended and applied to solve problems of more complex systems in the fields of supramolecular chemistry and the biosciences. The methodologies and the language developed will no doubt continue to assist scientists in different domains in the years to come. At present we can identify at least two fields of endeavor where the contributions of the physical organic chemist will be indispensable. These include the analysis of complex biosystems and the material sciences. Here I shall allude to the latter.

One may anticipate that the field of solids in general and the material sciences in particular will continue to be a central field at least in the beginning of the next century. Materials are a key technology for the development in a number of areas of pivotal importance in our daily lives. The systems to be dealt with in the future will become more and more complex and so it will force scientists of different fields to join forces in common endeavors. This should result in changes in many of the definitions of the scientific disciplines as we see them today. Many of the existing frontiers between chemists, physicists, biochemists, mathematicians, and engineers will be narrowed. Within certain fields, such as organic, inorganic, and physical chemistry, current barriers will be removed. Scientists will have to move more frequently from one field to another. However, whenever they attempt to address new scientific ventures they will have to rely on their previous experience and heritage. The methodologies developed by the physical organic chemists will acquire a pivotal position in the modern field of the material sciences. Among the main challenges of chemists and material scientists in recent years has been the replacement of empirical and semiempirical techniques for the preparation of functional materials by more rational methods of design starting from the molecular level. Materials of interest are composed generally of more than one component and a multitude of phases. The latter are generally separated by grain boundaries, dislocations, and defects. The structure of the molecules at these texture sites as well as their dynamics play at least as important a role in defining the macroscopic properties of the material as that played by the periodic structure of the composite. Therefore synthesis of such materials by design requires a knowledge of the structure and physical properties of the texture at a high degree of accuracy. One of the major tasks of the molecular scientists will be to invent the tools that will provide this knowledge.

Therefore one will continue to depend upon the development and adaptation of new analytical tools for the characterization of the stuctures and compositions of these hybrid materials on the one hand, and the design of new computational methodologies that link the atomic and molecular world on the other. The advent of synchrotrons, neutron reactors, intense lasers, more sophisticated scanning microscopes, near-field optical microscopes, x-ray photoelectron spectroscopy, solid state NMR and mass spectrometry of polymers, and electrochemical methods, to mention but a few, has revolutionized in recent years the field of the material sciences. With these tools in hand it became possible not only to characterize the structure of surfaces and interfaces but also to open new ways for design and study of nanostructures.

Current synthetic methodologies will be improved and new ones will be introduced. Larger and larger architectures will be created, going from the small to the large, and increasing in size and complexity. On the other hand engineering and lithography are moving from the macroscopic to the molecular, opening a new science of nanochemistry and nanotechnology. Design of luminescent solids for electro-optics and information storage will continue to receive particular attention. Techniques of molecular chemistry will be more extensively employed to assemble organic, organometallic, and inorganic blocks into magnetic molecular materials forming bulk magnets with permanent magnetization with high critical temperatures.

In spite of the intense research in crystal engineering, a comprehensive theory which links the constituent to the whole crystal is not available, and thus the design of a crystal with a desired architecture is still done by rule of thumb. Maddox, the editor of *Nature*, alluded to this inability by stating that the fact that one cannot predict the crystal structure of a simple organic molecule is one of the continuing scandals in the physical sciences. This problem will occupy presumably the best minds in years to come. The design of composites with a texture of a required structure will have to await the discovery of new synthetic methods. However, we may be optimistic that such goals should be achievable since Mother Nature has successfully fabricated during the years functional composites with unique physical properties. Biominerals such as teeth, shells, and bones with unprecedented strength were produced under physiological conditions. In recent years we have witnessed an increased interest in the study of the strategies adopted by organisms in building their skeletal hard tissues, in order to provide scientists with ideas for the production of sophisticated artificial materials. With the assistance of carefully designed biopolymers Nature has controlled the mechanical properties of biocomposites by controlling the structural and dynamic properties at the grain boundaries. Nature has applied also sophisticated control of the production methodologies rather than in the selection of the materials used for the production. In a different line materials scientists will continue to learn from Nature to construct new supramolecular architectures for the design of more complex functional devices such as efficient molecular and biomolecular sensors or for the preparation of biocompatible materials.

Optical and magnetic properties of materials at the level of micrometer dimensions depend on their size. Recently functional nanostructures have been prepared in a controlled mode by applying methods of layer by layer deposition. This includes coating surfaces by the Langmuir-Blodgett or self-assembling methods or by molecular beam epitaxy. The latter method is limited at present to simple inorganic thin films of galliun arsenate, indium phosphide, or organic thin films composed of very stable molecules such as the phthalocyanines. One may anticipate that these methods will be modified and expanded for other systems of interest. Changing the chemical and physical properties of surfaces in a controlled mode will continue to be applied in a large variety of fields such as heterogeneous catalysis, lithography, and in the optoelectronic sciences. Work on conducting, photoactive, and nonlinear optical organic polymers will proceed both in the theoretical understanding of these systems as well as in the search for more efficient ways to process these materials for the preparation of new optoelectronic devices in the preparation of molecular switches or for information storage.

Amorphous materials is another active topic of current research which plays an important role in a diverse range of applications such as optical fibres. Little is known about their structure and the short range order that govern their physical properties and that differ from material to material. New efficient ways to stabilize such materials and to prevent them from crystallizing will probably be discovered. Macroscopic properties such as wettability of surfaces, strain propagation in elastomers, friction between surfaces, viscosity of solids in viscous media, *etc.*, remain to be more profoundly understood at the molecular level.

Soft matter chemistry and physics is another subfield of the solid state sciences that will presumably continue to be active in the years to come. At the present time very little is known on the ways ionophores and channel forming materials transduce signals and ions through membranes. An intimate structural understanding of the changes that happen while these processes occur will probably result in the design of new and more efficient artificial membranes for separation processes or the desalination of sea water.

Finally theory, modeling, and simulation are now indispensable tools in material research and development, and will continue to assist the experimentalists in the preparation of the new materials.

In conclusion, a bright future is anticipated for the molecular scientists in the next century that will meet the old words of Gallileo, as stated in Dialogue (1632) "As to Science itself, it can only grow."