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Summary of the Proceedings of the Workshop on the Present Status and Future Developments of Solid State Chemistry and Materials

Arlington, Virginia, January 15–16, 1998

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INTRODUCTION TO THE REPORT

There is currently much discussion concerning the appropriate national paradigm for support of research. Accordingly, it seems important to evaluate recent advances and to articulate future challenges and opportunities in particular research areas. This is especially true of the rapidly emerging and changing field of solid state chemistry and materials which has undergone explosive growth, both in industrial and in academic laboratories, over the last decade. Part of this trend may be attributed to the discovery of new materials with important technological applications, and part of this is a reflection of the growth in intellectual scope of the field whose boundaries have expanded considerably: materials chemistry has emerged as a discipline in its own right, closely intertwined with activities traditionally recognized as being in the domain of solid state chemistry. It therefore appeared timely to institute a Workshop on the Present Status and Future Developments of Solid State Chemistry and Materials, to survey the many different activities in this field and to outline emerging and exciting trends, needs, and challenges.

The following guiding principles were adopted for the development of an agenda appropriate to a Workshop:

— Define research opportunities in the field of solid state chemistry and materials.

— Identify important multidisciplinary areas for involvement by the solid state chemistry and materials community.

— Determine novel roles for the solid state chemistry and materials community that will advance educational and training opportunities for future scientists, engineers, and technicians.

— Develop new approaches that allow for a more effective and efficient conduct of research and educational activities.

The Workshop was held January 15–16, 1998 at the NSF headquarters in Arlington, VA. Thirty-four individuals participated in various presentations; twenty-four registered individuals were in attendance as observers, and approximately thirty-five additional individuals, mostly NSF personnel, were present at various times during the Workshop. A very important component of the Workshop was the preparation of the Conference Proceedings as a report that received wide distribution. One of the aims of this document

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was to encourage continuing wide-ranging discussions of current advances and research opportunities in this area which is of great importance to our national welfare.

Appended to this Introduction is a Precis and an Executive Summary of the Workshop Report. Electronic copies (pdf files) of the complete Report may be found at the following web sites or by the pointers thereon:

http://www-chem.ucdavis.edu/groups/kauzlarich/dmr/
http://www.nsf.gov/mps/dmr/solid.htm.

Hard copies may be procured on request from Prof. P. K. Dorhout, Department of Chemistry, Colorado State University, Fort Collins, CO 80523–1872.

The full Report is meant to stimulate continuing community discussion and planning; the Workshop format is perhaps only one of several options under which such vital discussions can occur.

It should be emphasized that in the very limited time frame of the Workshop many of the present activities in areas that comprise solid state chemistry and materials activities could not be included. Several of these topics were covered in a Workshop on Interdisciplinary Macromolecular Science and Engineering, organized by S. I. Stupp, and held May 14–15, 1997, and in a Workshop on Materials Design and Processing at the Nano- and Mesoscales through Self Assembly, organized by M. V. Tirrell, held January 13–14, 1998. Therefore, the fact that these and several other ongoing research areas are not included in the Executive Summary or in the Workshop Report proper should not be construed as indicating that the Planning Committee considered them unimportant; some difficult choices had to be made. To deal with the omitted topics it is planned to convene additional workshops periodically, with complete rotation of organizing personnel, so as to minimize built-in prejudices that could hamper the free development of the field.

PRECIS OF WORKSHOP REPORT

A brief overview of some of the recommendations of the panel is provided below:

Many different innovative methods are presently in use to discover new materials by exploration of uncharted regions of thermodynamic stability or by materials processing in regions of metastability. Robot-assisted combinatorial synthesis is also being more commonly employed. Methods of choice for synthesis include templating, use of extreme operating conditions, low-temperature flux and hydrothermal techniques, self assembly, combinatorial chemistry, soft chemistry, and electrochemistry. Two strategies in use for discoveries are the chemistry-driven approach, concentrating on reactions, compounds, or structural motifs, and the properties-driven approach, emphasizing basic science or technological applications of materials. Both types of effort are required to advance solid state chemistry and materials research.

Theory will continue to be an important tool for the adjustment of variables that optimize characteristics, thus linking the synthesis of all types of materials with desired physical properties. Just as experimental data are currently used to model many physical properties, so theoretical calculations are expected to influence the generation of new materials and their properties. Tools available for this purpose and goals for successful implementation include user-friendly data bases, and the construction of quantum structure maps. Recommendations for the future include emphasizing the value of strong collaboration between theoreticians and experimentalists to resolve specific materials issues.

Education was given high priority in the Workshop. Many undergraduate students go through their curriculum without ever being introduced to the chemistry of extended structures. As a remedy it is important to include solid state chemistry and materials subject matter in elementary courses, train teachers to appreciate and foster the subject area, encourage interchange of resources and research capabilities among researchers in the field, and publicize by outreach highlights in the solid state chemistry and materials area.

Societal needs and technological opportunities may be addressed by understanding, controlling, and predicting properties of solids, so as to produce new materials with superior properties. Solid state chemistry and material activities have impacted on everyday activities in diverse areas such as health, energy, environment, electronics and communications, transportation, security, scientific breakthroughs, and education. Technologies dependent on a solid state chemistry and materials knowledge base are growing as fast as 50% per year, which requires a stream of steady solid state chemistry and materials research activities that largely evolve and grow in response to emerging technological needs. This calls for adventurous research activities, proper allocation of resources, skill sets that allow new knowledge to be acquired, and investigations into new areas. The U.S. ranks high in solid state chemistry and materials portfolios, but is seen lagging in fundamental research that produces new materials. Another danger signal is the scaling back of fundamental research in the industrial sector. Mechanisms to reverse this trend should be encouraged, and serious attempts should be made to remove obstacles, such as limiting intellectual property rights. Steps such as providing sabbatical leaves of absence, encouraging scientific exchanges, and instituting more tutorials are also important in redressing the problem.

Materials chemistry is also playing an increasingly important role in our technological society, especially in the production of materials by the major chemical companies in the U.S. Academics, through their activities in interdisciplinary, frontier-type research, and through availability of increasing funding in this area, can be expressed to become involved in the industrial development of new materials; the NSF should provide a leadership role in this important domain. This type of collaboration would also address societal needs and technological opportunities. The explosion of information in response to technological needs calls for adventurous research activities and for renewed support by industry of fundamental research activities.

EXECUTIVE SUMMARY

Structure–Property Relationships—S. Lee

Computer-based calculational projects form an important tool for the adjustment of variables that optimize characteristics linking the synthesis of all types of materials with desired physical properties. Tools available for this purpose and goals for successful implementation include:

— User-friendly data bases (enumerated in the text) which survey compounds, reactions, physical properties, and structures, complete with codes that allow processing and statistical studies.

— The construction of quantum structure maps, based on atomic parameters, as a function of composition; these are useful for the prediction of the existence of new phases and of their properties.

— Theory and computation. Just as experimental data are currently used to model many physical properties, so theoretical calculations are expected to influence the generation of new materials and their properties.

— The development of interconnective information encompassing virtually all steps in materials development. More collaboration between theorists and experimentalists is expected to strengthen this very important process.

Density functional theory is a very important tool in the achievement of the above-mentioned goals. Of great value would be improvements in the empirical and semiempirical methodologies appropriate to the analysis of very large collections of atoms that begin to simulate the solid state. A listing of factors involved is found in pdf format at http://www-chem.ucdavis.edu/groups/kauzlarich/dmr/NSFWork98.pdf (Table 1, p. 17). Problems considered heretofore as inaccessible have now become tractable; a listing is provided in the text.

Recommendations for the future include emphasizing the value of strong collaboration between theoreticians and experimentalists to resolve specific materials issues. Experimentalists should be assigned in learning how to do their own calculations rather than relying exclusively on theoreticians. Toward this goal it is necessary to develop more user-friendly codes, organizing tutorial workshops, and making supercomputing facilities more readily available to nonspecialists.

Discovery of New Materials—R. Cava

Many different innovative methods are presently in use to discover new materials by exploration of uncharted regions of thermodynamic stability or by materials processing in regions of metastability. Robot-assisted combinatorial synthesis is also being more commonly employed. Methods of choice for synthesis include templating, use of extreme operating conditions, low-temperature flux and hydrothermal techniques, self assembly, combinatorial chemistry, soft chemistry, and electrochemistry. The creative use of such techniques is well illustrated by the world-wide research and development efforts in the area of high-temperature superconductors.

Two strategies in use for discoveries are:

— The chemistry-driven approach, which concentrates on reactions, compounds, or structural motifs, with lesser emphasis on properties.

— The properties-driven approach, with emphasis on basic science or technological applications of materials, with the goal of optimizating their properties.

Both types of effort are required to advance solid state chemistry and materials research.

New materials, such as the high-temperature superconductors, lead the way in technological progress, revealing new phenomena and/or forcing a reevaluation of what was thought to be understood. A listing of such materials discovered in the last 25 years is supplied in the Report; the obvious high degree of interest and activity in this area continues unabated. It is therefore important to encourage further active research leading to the discovery of new materials. A vast area is still unexplored; for example, only 0.01% of all possible quaternary intermetallic compounds have so far been investigated. Maintenance of core expertise in such an endeavor is absolutely essential, with particular emphasis in following up new leads as these arise.

As also emphasized elsewhere, a high degree of interdisciplinary effort should be encouraged to attain the above goals, centered on the training of students in areas outside the normal chemistry curriculum. NSF should be encouraged to expand focused research programs that involve solid state chemistry interacting with contiguous disciplines. The successful establishment of such programs in academia should be recognized as an important consideration in tenure decisions at universities.

More effort should be placed on the synthesis of new materials by design, rather than on finding out what materials can be made. This requires more studies on reaction mechanisms, as well as computer-aided methodologies which can predict properties from first principles. As also stated elsewhere, user-friendly computer programs will greatly assist in this task.

Hybrid Materials—M. D. Ward

Hybrid materials play an increasingly dominant role in the synthesis of future products generated through solid state chemistry and materials research and development. A major problem in this development is the proper control of interfaces separating dissimilar components. Thus, future solid state chemistry and materials research must adequately deal with new interface design principles and with the development of functional molecular entities capable of controlling interfacial properties. This also requires structure and property design at small length scales, so as to achieve complex hierarchical structures at large length scales. Examples of emerging activities include thin films structures, layered compounds, as well as three dimensional crystalline and disordered networks. Synthetic methods generally involve the "bottom up" approach by: (a) deposition of films, (b) use of molecular building blocks for synthesis of self-assembled monolayers, (c) sol–gel synthesis, (d) organic structure or surfactant-directing agents, and (e) use of colloid chemistry and intercalation. In these activities templating provides exquisite control over synthesis of hybrid materials with desired properties. Such operations are generally carried out under conditions far removed from equilibrium at low temperatures, to ensure stability.

The above operations require characterization capabilities with a new generation of tools capable of operating in the microdomain, especially microscopic imaging and tomography, probing buried interfaces, developing new methods for detection of defects and trace analysis, and developing user-friendly theoretical tools for modeling interfaces. Future challenges include the establishment of structure–property relationships involving several length scales, studies of noncovalent forces governing interfacial structures, learning how to control interfacial stability, developing better computational strategies, and systematic development of new materials.

Societal Needs and Technological Opportunities—D. W. Murphy

Societal needs and technological opportunities may be addressed by understanding, controlling, and predicting properties of solids, so as to produce new materials with superior properties. Solid state chemistry and materials activities have impacted on everyday activities in diverse areas such as health, energy, environment, electronics and communications, transportation, security, scientific breakthroughs, and education. We depend both on sudden burst of insight and on logical extension of current technologies to attend to societal needs.

Technologies dependent on a solid state chemistry and materials knowledge base are growing as fast as 50% per year, which requires a stream of steady solid state chemistry and materials research activities that largely evolve and grow in response to emerging technological needs. This calls for adventurous research activities, proper allocation of resources, skill sets that allow new knowledge to be acquired, and investigations into new areas. The U.S. ranks high in solid state chemistry and materials portfolios, but is seen lagging in fundamental research that produces new materials. Another danger signal is the scaling back of fundamental research in the industrial sector. Mechanisms to reverse this trend should be encouraged, and serious attempts should be made to remove obstacles such as limiting intellectual property rights. Steps such as providing sabbatical leaves of absence, encouraging scientific exchanges, and instituting more tutorials are also important in redressing the problem.

A detailed listing of representative accomplishments and opportunities in the solid state chemistry and materials area is furnished (Table 4, p. 51), in the body of the report.

Panel on Education—S. M. Kauzlarich

Many undergraduate students go through their curriculum without ever being introduced to the chemistry of extended structures. As a remedy it is important to:

— include solid state chemistry and materials subject matter in elementary courses,

— train teachers to appreciate and foster the subject area,

— foster interchange of resources and research capabilities among researchers in the field,

— publicize by outreach highlights in the solid state chemistry and materials area.

Listed in the body of the report are a number of NSF-sponsored educational projects which the Panel identified as having been highly successful at the K–6 grade level, the middle and high school range, and for the college curriculum; most relevant and notable among these is the Summer Research Program in Solid State Chemistry for Undergraduate Students and College Faculty, which was been highly successful. Materials intensive courses are identified in the main body of the report, as well as instructional materials, appropriate resource articles, models, and the like. The Panel also provided information on (a) instructive articles in the related areas of polymer and materials science, (b) listings of research efforts in these areas, (c) descriptions of research opportunities in these fields, and (d) the present status of the initiation of the IGERT program at NSF.

The Panel further issued several recommendations:

— Guidance should be provided to prospective students in the solid state chemistry and materials area through workshops, textbooks, American Chemical Society-certified courses, team-taught instruction, and Ph.D. programs specific to the area.

— Special curricula should be set up emphasizing undergraduate research programs that are supervised by small collaborative teams of faculty in different departments or even different campuses.

— Current NSF-sponsored research should include an educational component.

— The solid state chemistry and materials activities should have wide representation at national meetings of professional societies through plenary lectures and tutorials involving cutting-edge work in the field.

— A web site should be instituted on teaching resources, as should faculty web sites, research and co-op opportunities and fellowships, and research interactions between faculty and personnel in national laboratories.

— An effort should be made to provide the public with better information of activities in the solid state chemistry and materials area through articles, other means of information dissemination, and involvement in local school science projects.

Panel on Facilities and Resources—T. M. Swager

In its meeting the Panel dealing with Facilities and resources commended NSF for effectively promoting science and innovation with limited resources. The overall consensus is that the Division of Materials Research maintains a multifaceted portfolio that is responsive to scientific needs and opportunities. Changing times have required new mechanisms for supporting young faculty (CAREER), support for interdisciplinary research teams (STC and MRSEC), funding exploratory research (SGER), and increased equipment resources. The balance of these programs is considered to be carefully managed so as to produce the maximum impact from NSF dollars. The Workshop participants felt that the average grant size should not be increased if this leads to a reduction in the number of individual grants, for which the success rate is already dangerously low. This community also favored a mail review system in which reviewers are asked to handle proposals in batches, so as to provide a basis for comparison of the relative merits of different proposals in the same area. While no specific redistribution of funds in DMR were recommended, the Workshop participants and the members of the facilities and resources panel voiced strong support for some particular initiatives. DMR's recent success in effectively doubling the IMR budget was warmly appreciated, and is a proper response to the ever expanding role of sophisticated equipment and facilities in the execution of materials research.

The Workshop participants further felt that there was a reasonable balance in the allocation of funds to large research centers and individual researchers. However, information concerning access by outsiders to work station at various centers should be made more readily available to the community at large than is presently the case. The Workshop panel and the participants examined presently available large scale sophisticated equipment and identified further opportunities for equipment initiatives, including complex synthesis equipment (furnaces, molecular beam epitaxy, etc.), facilities for combinatorial materials synthesis and screening, high-field (900 MHz) NMR, and equipment for the characterization of materials under extreme conditions (high/low temperatures, high pressures).

The possibility of creating remote access capabilities that directly tie into research centers should be carefully examined and then implemented. A new initiative should be pursued which allows individual scientists to purchase modern equipment too costly to be included in standard grant proposals, and yet not large enough to qualify for the current equipment grant proposal. This is deemed to be important because of increasing needs for sophisticated equipment of this type in the laboratory of individual researchers.

The Workshop community also supported the establishment of a postdoctoral fellowship program in DMR, which would assist in the training of future researchers. The panel felt that an expansion of cooperative interagency agreements would represent an important opportunity for graduate fellowship support. Mechanisms for the more effective utilization of DOE and NIST facilities in NSF sponsored research should also be investigated.

Panel on Defining What Is Materials Chemistry—S. I. Stupp

A panel was organized to pose and address the question "What is the intellectual scope of materials chemistry?" through interactive discussion. It was also of interest to this panel to establish the relations between materials chemistry and other well established disciplines, such as chemistry, materials science, chemical engineering, and solid state chemistry. Materials chemistry is generally taken to be a discipline concerned with the understanding and control of functional condensed matter from a chemical perspective.

Materials utilized by society need to be processed into macroscopic functional forms; their chemical nature and complexity will evolve over time. Therefore, practitioners of materials chemistry must have growing interactions with all disciplines of chemistry and with other fields of science and engineering. These interfacial, interdisciplinary efforts are currently experiencing rapid growth. There is also general agreement in the community that materials chemistry is an exciting area of scientific opportunity that will profoundly affect our increasingly technological society. Its importance is clearly demonstrated by such trends as the increasing number of journals and publications in materials chemistry, by the increasing number of faculty who are involved in materials research, by the growing interest of funding agencies in the welfare of the field, and by the materials chemistry materials produced by the top 100 chemical companies in the U.S. The top six of these companies have presently a significant stake and interests in materials; the number of companies among the 100 whose products are mainly related to materials chemistry can be estimated conservatively to be as high as one third. In terms of chemical sales the majority of these companies rank among the top fifty. In light of the above, academics can play a very useful and supportive role in the industrial development of materials chemistry, and NSF should provide adequate support of research and foster industry–academic cooperation in this area.

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