Membrane Science Workshop at the APS: Report and Recommendations

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This is a brief summary of the "Workshop on Membrane Science," August 17-18, 2004, Argonne, IL, which explored the future scientific directions with the unique capabilities provided by high-brightness, high-energy synchrotron-radiation facilities, such as the Advanced Photon Source (APS) at Argonne National Laboratory.

The focus of the workshop was on the emerging research topics in membrane science. These are truly interdisciplinary and represent the interfaces among chemistry, materials physics, molecular biology and medicine. For example, inorganic membranes, owing to their thermal, mechanical, and chemical stability, have been used in many industrial separation processes. Organic membranes are used for a variety of liquid and gas-phase separations and for the extraction of trace organic pollutants from water. The supramolecular architecture of biological systems is based on ultra-thin and highly flexible bio-membranes. Most bio-membranes exhibit a universal construction principle: a self assembled bilayer of lipid molecules with many anchored macromolecules. Understanding chemical ordering, pattern formation, kinetics, and dynamics in organic and inorganic membrane structures, as well as the physical interactions between bio-membranes and supramolecules, their dynamics under stimuli, and the formation and structure of ion channels in these bio- membranes formed the basis for discussion at this workshop.

The workshop emphasized the need for fundamental structural understanding to control the formation of membranes on all length scales (molecular, nano, micro, and macro) whether the membranes are fabricated or self-assembled. It is even more challenging to create new types of so called bio-inspired membranes without utilizing the insights obtained by studying biological structures. The new synthesis processes are driven by potential applications where the membrane properties and function are to be integrated from the molecular scale to the macro-scale, which span 7-8 orders of magnitude in length and time scales. The workshop identified key problems where the application of x–ray analytical tools will enable significant progress in relating structure and function. Towards this goal it is necessary to determine high-resolution membrane structures in one-, two-, and three-dimensions in the molecular-, nano-, micro-, and macro-scales, and to perform element-specific mapping of real-time information on the kinetics and dynamics in the membranes on multiple scales.

The growing application of membrane technology in modern industrial processes has made it an integral part of many corporate and national (e.g., DOE, NSF, NIH) R&D

programs. Membrane based technologies have advanced the state-of-the-art in areas of water treatment and production, niche applications in the electronics, semiconductor, chemical, petrochemical and pharmaceutical industries as well as environmental control. New research opportunities range from controlling the medical and biological processes, such as hemodialysis found in artificial kidneys or the separation of proteins and microorganisms, to providing essential components for fuel cell and hydrogen energy economy and technology. All these examples were well represented by the leaders in these areas at the workshop.

A successful hydrogen-economy based on fuel cells to power cars, truck, homes and businesses will require advances to be made in key technology areas. Among different types of fuel cells, the most useful for vehicle transportation will be proton exchange membranes (PEMs) because they operate at relatively low temperatures. It was clear from workshop discussions that further research is needed in identifying new membrane materials with better efficiency to make them cost effective and the structural information is the key towards this goal.

Membrane filtration at micro- and nanoscale is also used for the separation of proteins in food, beverage, pharmaceutical and biotech industry. Within pharmaceuticals and biotech, membrane filtration is increasingly the method of choice for separating amino acids, enzymes, yeast, insulin, ferritin, glycoproteins and biopesticides from proteins. Membranes will play a major role in the recovery, isolation and concentration of these proteins.

Membranes have been prepared with increasing sophistication to meet newer challenging applications, and commensurately scientists have refocused on the fundamental questions regarding their properties and performance. Some of these questions have become more complex having to address physical, chemical and biological properties and interactions at microscopic, nanoscopic and atomic scales. Detailed understanding of these questions has demanded new experimental tools and theoretical models. Many experimental probes and techniques, such as laser spectroscopy, electron spin resonance, nuclear magnetic resonance, neutron scattering, Raman spectroscopy, electron microscopy, and computational modeling, can currently provide information bearing on the questions of interest. However, the diversity of interactions among molecules with membranes discussed at the workshop require probes that are sensitive to the local and extended atomic and electronic structure, as well as to the geometric structure in membrane interfaces with solids, liquids and gases over a wide range of spatial and temporal dimensions. Both lateral and vertical (depth) dimensions must be probed. During the last decade, techniques based on synchrotron radiation, such as wide-angle x-ray scattering (WAXS), small-angle x-ray scattering (SAXS), ultra small-angle x-ray scattering (USAXS), grazing-incidence small-angle x-ray scattering (GISAXS), x-ray reflectometry (XRR), diffuse x-ray scattering, x-ray photon correlation spectroscopy (XPCS), grazing-incidence x-ray diffraction (GIXD) and x-ray absorption spectroscopy (XAS) have been shown to provide unique structural information at molecular level on membranes, its interfaces and interacting supramolecules. These techniques in the real-time domain give further insight into time evolution and molecular interactions in these systems. Together these capabilities have clear potential to impact the future scientific directions for this field and perhaps begin to address some of the unanswered questions.

The workshop participants were unanimous in their recommendations and excitement of the potential use of the APS in membrane science research. It was viewed by the workshop participants that the APS is one of the leaders in the world in this research and they made the following critical recommendations for the APS to maintain the leadership role in the rapidly growing field of membrane science:

1. The APS must maintain the successful scientific environment that both enables and enhances experiments using various x-ray tools mentioned above.

2. Potential ground breaking research in future (nucleation, growth, dynamic self-assembly, molecular interaction, etc.) require *in situ* investigations in unusual experimental environments capable of concurrently performing x-ray scattering as well as other optical and thermodynamic measurements. APS should aggressively work with science leaders in this field to develop such capabilities and make them available at the beamlines *dedicated to membrane science*.

Both these goals can be best achieved by forming a *'membrane science advisory panel'* to interface with the APS to develop a plan to: 1) optimize and refurbish existing beamline capabilities and infrastructure to support membrane science experiments at a select set of beamlines, 2) hire resident scientific staff with experience and interest to provide leadership to the user community in the field of membrane science, 3) provide a *new dedicated* bend-magnet beamlines with suitable x-ray optics, end-station instruments and 2-D detectors (including various experiment environments and auxiliary non-x-ray tools), 4) provide modeling and simulation capabilities to perform in-line data analysis. It was also recommended that since there is a potential for bringing many new users to the APS, a workshop on the use of x-ray tools for membrane science research, with hands-on training for the workshop participants, be held as early as possible. Also a 'Membrane Science Interest User Group' will be formed at the APS which will regularly meet and at the APS Users' Meetings. The 'membrane science advisory panel' will receive its input at these meetings of membrane science users.

These recommendations were designed to effectively enhance existing capabilities of the APS and to build new dedicated beamline with unique capabilities for frontier membrane science; develop infrastructure/technology to make the auxiliary tools along with the x-ray tools available for performing *in situ* membrane science research more broadly; and expand the capacity of membrane science experimentation at APS to support anticipated new users who were present at the workshop. Finally, the present and future scientific users in the membrane science field who participated in the workshop were eager to be fully involved in the implementation and success of both of these recommendations.