Research Frontiers
FOR THE CHEMICAL INDUSTRY

report on

THE FOURTH ANNUAL
CHF–SCI INNOVATION DAY
WARREN G. SCHLINGER SYMPOSIUM

INNOVATION DAY 07

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11 SEPTEMBER 2007

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Innovation Frontiers in Industrial Chemistry

A Report on the Fourth Annual
CHF-SCI Innovation Day
11 September 2007

INTRODUCTION

Innovation is inherently a social process—an activity performed by human beings and embedded in a particular time and place as part of an intricate network of disparate institutions. The driving force for technological innovation comes, frequently but not exclusively, from the pressures that shape real and perceived societal needs. Successful innovation is characterized not simply by invention, but by an ability to successfully intermesh new ideas or methods with social context, to implement them and make them real. Because successful innovations enter society through diverse pathways, they often bring about an unexpected reconstruction of the social milieu. And once entrenched, successful innovations tend to become inextricably linked with that social world, making the possibility of extraction increasingly difficult.

Take, for example, the development of the recyclable/disposable water bottle. Cheap, portable water has become a mainstay of emergency relief efforts and signaled an important switch in everyday consumption habits, with consumers exchanging their soda bottles for water bottles. But cities have balked at the growing number of water bottles filling their landfills (instead of recycling centers) and sewers (especially in the wake of large public gatherings). The water bottle has become a facet of contemporary culture, however, and it has been hard to extricate, even in the face of mounting criticism.

What then are some of the imminent social pressures we face today? In past reports in the series Research Frontiers for the Chemical Industry, we have pointed to the juggernaut forces of globalization, increased attention to global climate change, and the urgent need to remain competitive and innovative in the crowded marketplace. These pressures remain strong today; some are even stronger as the price for crude oil has hit record highs, hovering above $140 per barrel (as of this writing in mid-July 2008). This situation might be reason enough to pique the chemical industry's interest in getting serious about a more diversified chemical feedstock stream and a continued search for alternative energy sources. Faced with these challenges, past reports have argued, chemical companies would need to pay closer attention to cooperative ventures—with corporate, noncorporate, and academic partners—in areas with long-term implications.

While this report largely echoes what has been discussed in the past, it adds another dimension: complexity. As technological innovations go through the complicated process from conception to implementation, things often do not turn out the way that their proponents originally intended. Take for example the recent controversy over biofuels in light of soaring food prices in the global marketplace. In June 2008, after three days of intense debate at the Food Security Summit sponsored by the United Nations, world leaders failed to reach a consensus about the overall impact biofuels are having on this situation, leaving the meeting with a declaration simply calling for a "more in-depth study." Nevertheless the stalemate at the summit indicates the drastic turn of fortune for biofuels research and development: very recently touted as a sustainable fuel supply for the future, biofuels are now being singled out as the key culprit for the global food crisis. This turn of events brings into sharp relief the complexity and global nature of contemporary technological innovations. In this climate, problems have no absolute solutions, partly owing to the complex dynamics of technical and social changes.

With expanding frontiers in industrial chemistry—both in terms of knowledge and geography—the complexity is bound to increase. While this shift will, quite literally, produce more opportunities, it will also introduce a higher level of uncertainty into corporate decision making. The factors that will raise the level of ambiguity are multifarious: what will be the impact of the growth of China, India, and other emerging or expanding economies? How can a U.S. firm operate efficiently in these unfamiliar geographical and cultural environments? What is the best way to forge links among diverse sets of institutions, both private and public, to form networks for sustainable chemistry and engineering? Will the adoption of solar energy as an alternative energy source lead to a net benefit in our energy consumption? Will further miniaturization of microchips come to an end within the foreseeable future, and what can the chemical industry do to prepare for the impending paradigm shift? These challenges are a small portion of those lying ahead for the chemical and molecular-science industries. To understand the role that these and other factors will play in the formation of a twenty-first-century global chemical industry, we must begin exploring the ways in which these forces of change are converging.

The purpose of the CHF-SCI Innovation Day and Warren G. Schlinger Symposium is to expose young investigators in the chemical and molecular-science industries to issues on the cutting edge of the innovation frontier. In this age of complexity and global interconnectedness, it is no longer sufficient for industrial chemists to concern themselves only with technical matters. Being aware of the broader implications of their work will become increasingly critical for continued success. In that regard the proceedings of the annual Innovation Day provide a unique opportunity for young industrial chemists to take a step back from their day-to-day operations to contemplate the bigger picture, expanding their outlooks into the broader social, economic, and political contexts that impinge upon contemporary innovative activities in the chemical and molecular-science industries.

FRONTIER AREAS FOR INDUSTRIAL CHEMISTRY

At the core of the Innovation Day proceedings are conversations captured during six breakout sessions that serve as incubators for more in-depth discussions. The session topics and speakers are selected by the Innovation Day Steering Committee, composed of chief technology officers and top scientists of leading chemical companies. In 2007 the breakout sessions covered the following topics:

1. Eco-Friendly Products
2. Sustainable Chemistry and Engineering
3. Health Materials
4. Chemistry of Energy Sources
5. Electronic Materials
6. Emerging Global Economies

Rather than reproduce the presentations, in what follows, we attempt to offer a sense of the conversations that took place, guided by session presenters but participated in by all present.

ECO-FRIENDLY PRODUCTS

Moderator: *Ryan R. Dirkx (Arkema)*
Speakers: *Terrence Collins (Carnegie Mellon University)*
Carina Maria Alles (DuPont Engineering Research and Technology)

In this age of ubiquitous eco-marketing, the burning question is what makes a product eco-friendly? While everyone might agree that eco-friendly is a good thing, there seems to be little consensus on its definition. Looking at the trajectory of the chemical enterprise from a long-term historical perspective, industrial chemists have created roughly 80,000 commercial chemicals since Sir William Henry Perkin synthesized the first aniline dyestuff in 1856. Nevertheless, only during the last few years have we begun to recognize the profound impact that these new chemicals might have on the environment or health. In other words, questions about toxicity and eco-toxicity have not been asked during the innovation process of many new chemical substances.

The two speakers at this session focused on the "life cycle" of particular chemical substances, moving from the innovation process to synthesis in the laboratory, production, consumer use, and beyond. Terrence Collins, Thomas Lord Professor of Chemistry and director of the Institute for Green Oxidation Chemistry at Carnegie Mellon University, emphasized a "holistic" approach in developing and introducing new chemical substances to the environment. This approach, broadly associated with green chemistry, advocates a cognitive shift from *design for* to *design against*. In other words, rather than allow economic factors to be the main driver of chemical innovation, the holistic approach takes into account various environmental and health consequences in order to design against such potential risks. In order to accomplish this cognitive shift, Collins called for two changes. The first requires chemistry curricula to include topics of ethics, green metrics, historical sensibilities, and a focus on potential risks. The second called for aligning various social determinants—such as government policy and business mindsets—to address ecological concerns that stretch beyond the current generation.

Carina Maria Alles, group leader of Engineering Evaluations and Sustainability at DuPont Engineering Research and Technology, further elaborated the ways in which industrial chemists can fundamentally reengineer the processes by which current products are designed. Like Collins, Alles focused on the role that life-cycle analysis can play in developing genuinely eco-friendly products. In order to better understand and measure the "greenness" of a new product, analysis of the entire life cycle of the substance from a molecular level—including production, use, and disposal—is necessary. Ideally eco-friendly products should strive to meet three criteria. First, they should be of equal or better quality than the products they are replacing. Second, they should reduce the overall product footprint in energy consumption, resource depletion, and emissions. Finally, they should be susceptible to eco-friendly disposal practices, meaning they can be reused, recycled, or safely disposed.

Taking these holistic approaches into account will have profound implications for our decision-making processes. How should we integrate considerations of toxicity into our thought process as we continue to develop new chemical substances? What are the conditions under which there will be a net-energy benefit to adopting, for example, photovoltaic solar cells as an alternative energy source? These considerations not only provide the framework to challenge conventional wisdom; they also remind us of the inherent complexity and uncertainty involved in contemporary innovation processes.

SUSTAINABLE CHEMISTRY AND ENGINEERING

Moderator: *Miles Drake (Weyerhaeuser Company)*
Speakers: *Henry C. Foley (Pennsylvania State University)*
Paul Bryan (Chevron)

As the concept of sustainability has entered the common vernacular in recent years, scientists and engineers have begun to explore the ways in which current industrial practices may be contributing to global ecological problems as well as the ways in which new practices can be developed to promote a sustainable society through chemistry. Though defining exactly what is meant by such terms as *sustainability* remains an ongoing debate, the reality is that many institutions, including private enterprises, universities, and national laboratories, have embraced the concept and have begun to exploit its potential for guiding research and energizing a new generation of scientists and engineers. Participants in this breakout session discussed cross-fertilizations between various institutions and subsequent efforts to create and promote a sustainable chemistry.

Henry Foley, dean of the College of Information Sciences and Technology at Pennsylvania State University (PSU), presented the perspective of the land-grant university and its attempts to transform institutions to meet the needs of the twenty-first century. Major forces that drive such transformations are international economic development, national security (especially dependence on foreign oil), environmental change (most notably, global climate change), and diminishing resources (as powerfully forwarded by the Hubbert peak theory, which states that the rate of petroleum production has a tendency to follow a bell-shaped curve). Foley focused particularly on the ways in which institutions can help our energy challenges, and identified gaining a full understanding of the complex system that comprises the production, distribution, and maintenance of the global energy infrastructure as the first step toward redesigning the current system.

In order to meet these challenges PSU has established five new research centers, housed under an umbrella organization called the PSU Energy Institute (http://www.energy.psu.edu), to create an integrated energy research portfolio: the Hydrogen Research Center; Electrochemical Engine Center; Pennsylvania Transportation Institute; Center for Metallobiochemistry; and Biomass Energy Center. Through this network of research initiatives, PSU aims to integrate fundamental science, innovative engineering, and practical impact in the field of energy. This project involves not only employing cutting-edge science and technology but also creating a pipeline of energy-related educational initiatives across disciplines at both the undergraduate and graduate levels. Moreover the PSU initiative is an attempt to continue its tradition of providing engineering extension services to the local community as a land-grant institution. By engaging government and industry partners PSU is establishing a new model for public universities to make inroads into one of the more urgent problems in the twenty-first century.

Paul Bryan, vice president of biofuels technology at Chevron, also spoke about the energy crisis, noting the ways in which global energy issues are also global chemical issues. As PSU is making links with governmental and industrial organizations, Chevron is experimenting with new corporate and academic alliances in the field of biobased feedstocks. Biomass comes with a host of concerns, including seasonality, momentum of existing infrastructure, crop fluctuation, land availability, and competition with food. Nevertheless, the new network model of R&D (as opposed to conducting all aspects of R&D in-house) has provided Chevron with valuable organizational experiences by creating new access to expertise, providing training for the company's researchers, and producing opportunities to observe different cultures, industry segments, and organizational types.

The experiences of PSU and Chevron show that paradigm-shifting transformations in established scientific, engineering, and industrial practices cannot be achieved by a single organization. They necessarily require cooperation and alliances among different kinds of institutions, including universities, private companies, and government laboratories. Only through efforts that span the spectrum of organizations can we expect fundamental breakthroughs that show a glimpse of an alternative, sustainable future.

CHEMISTRY OF ENERGY SOURCES

Moderator: *Michael Altes (Dow Corning Corporation)*
Speakers: *Charles F. Gay (Applied Materials)*
Stanley R. Bull (National Renewable Energy Laboratory)

As discussed in the breakout session on sustainable chemistry and engineering, energy issues have been at the fore in industrial chemistry for some time now. Many scientists, engineers, and policy makers have proposed ways to make the transition to alternative energy sources, including wind, solar, and biomass. The chemical and molecular-science industries face dual motivations on this front. On the one hand the industrial establishment has a tendency to maintain the status quo; on the other hand the chemical sciences have the potential to solve many of the biggest materials challenges involved in the creation of alternative energies. Many seem to agree that the greatest barrier preventing the adoption of alternative energy sources is the lack of a coherent national, state, and local energy policy and strategy. With their technical and political muscle, the chemical science–based industries have an opportunity to help establish a coherent framework to make these changes possible.

Stanley R. Bull, associate director of science and technology at the National Renewable Energy Laboratory, addressed the role of chemistry in energy sources. The U.S. Department of Energy is currently engaged in a number of energy-related projects under the rubric of the Advanced Energy Initiative, including solar, biorefining, wind, and hydrogen, and chemistry will continue to play a critical role in producing all alternative energy sources under consideration. Bull singled out wind energy as the most cost-competitive source other than petroleum. Indeed, the General Electric Company is developing offshore turbines with blades the size of a 747 jet, which will be able to generate electricity in a relatively cost-effective fashion. One of the key challenges with wind energy is producing materials for the blades that will allow enhanced efficiency and resistance to harsh environments; with solar energy the chemical challenge is to create a high-temperature heat-transfer fluid for parabolic-trough electricity generation; with biomass the challenge is to develop a practical conversion process for each biomass feedstock. Naturally, these are but a small slice of the massive challenges in the field of energy sources that the chemical and molecular-science industries are facing.

From the industry perspective Charles F. Gay, corporate vice president and general manager of the Solar Business Group at Applied Materials, discussed how a traditional semiconductor equipment firm is expanding its reach into the field of solar energy. There are two methods of manufacturing photovoltaic (PV) cells. One uses crystalline silicon, adapting integrated-circuit techniques to PV. This technique is more appropriate for smaller-scale residential applications, and the key challenge is to increase the throughput in the manufacturing process. The other is the thin-film approach, related to display technology. This approach is more suited to large-scale applications, and the key challenge is to scale up the devices using larger glass substrates. The cross-fertilization of the semiconductor industry and photovoltaic industry has yielded some fruitful results. Currently the trade association Semiconductor Equipment and Materials International is one of the most vocal advocates of the PV industry. As of 2006 more silicon was used for PV manufacturing than for integrated-circuit manufacturing.

The case of Applied Materials illustrates that it is indeed possible for PV to enter the stage of industrial development that integrated circuits have occupied for the last forty years or so. With continued innovation PV cells might show an exponential dip in cost per watt, as we have seen in the Moore's law curve. Government interventions in the form of subsidies, tax incentives, and other regulatory devices will provide the rules of the game. Equally important, however, will be the continued innovations that are likely to arise as a result of cross-industry fertilizations among advanced materials, semiconductors, and the chemical industry.

HEALTH MATERIALS

Moderator: *William Fraser (The Dow Chemical Company)*
Speakers: *Leonard J. Buckley (Naval Research Laboratory)*
Angelo G. Scopelianos (Johnson & Johnson)

Defining the boundaries of the health-materials sector is a challenge, given that it encompasses items from medical devices to such vanity products as cosmetics. Therefore tackling the panoply of problems arising within the field of health materials requires close interaction among disciplines that include biology, chemistry, physics, engineering, materials science, and medicine. Within this broad purview the speakers for this breakout session focused on nature as an important partner for innovation.

Leonard J. Buckley, head of Materials Chemistry Research at the Naval Research Laboratory, discussed the ways in which innovation in health materials can be inspired by nature. "Bio-inspired innovation," in Buckley's words, includes self-decontaminants (or self-cleaning surfaces) inspired by the lotus leaf and graded index lenses inspired by fish eyes. Apart from these colorful examples, there are numerous lessons to be learned by closely observing how nature operates, as in research for new natural pesticides and fungicides. While the study and emulation of natural organisms might be a fertile area and methodology for advanced materials research, biological processes usually take a long time, which might be a resistance factor for human emulation. Industrial chemistry must overcome the time challenge as it considers bio-inspired materials innovations.

Angelo G. Scopelianos, vice president for R&D at Johnson & Johnson, emphasized the major advances in health materials during the recent past, especially in the fields of biomaterials and medical devices. Continued innovations in biomaterials have dramatically increased life expectancy. The main driver in innovation is customer needs. Permanent devices have made way for absorbable devices using bio-friendly composites. Traditional tissue engineering is slowly moving toward tissue regeneration, paralleling the broader trend of regenerative medicine. The push toward smaller devices also calls for further miniaturization. These challenges ultimately require the convergence of, and collaboration among, multiple scientific and technical disciplines to come up with solutions for particular problems confronting the industry.

These cases elucidate the complexity and higher level of standards inherent in health-related innovations. Health materials require a comprehensive set of experiments and testing to ensure that new materials will be safe when introduced to the human body. This emphasis on safety is certainly not the case in many other commercially oriented sectors, where time to market and cost are the main measurements for gauging innovations. Industrial chemists engaged in the health-related fields are, therefore, more likely to take a cautionary approach in introducing new innovations, such as imitating nature. This approach might be seen as inherently conservative; but recent developments show that bio-inspired technologies can yield exciting and ingenious innovations in the critical field of health materials.

ELECTRONIC MATERIALS

Moderator: *Gary Calabrese (Rohm and Haas Company)*
Speakers: *Sharon L. Nunes (IBM)*
Rajarao Jammy (Sematech)

The statement that Moore's law represents the fundamental dynamics of the semiconductor industry's "technology treadmill" has become a cliché. Nevertheless while prominent device manufacturers like Intel and National Semiconductor receive the spotlight, equipment and materials firms, which enable the industry to stay on track, are largely ignored. This discrepancy was the focus of the electronic materials breakout session. As chip manufacturing grew increasingly complex in order to keep up with Moore's law, an entire subsector of the industry specializing in electronic materials had to be mobilized to supply manufacturers with the specialty materials required for chip fabrication, including materials for packaging, display, connectors, and chemical mechanical planarization.

Since the early 1990s the trajectory of Moore's law has been governed by a group of industrial leaders at Sematech, a government-funded industry consortium devoted to semiconductor manufacturing. Sematech has been the home for the International Technology Roadmap for Semiconductors. Rajarao Jammy, director of the Front End Processes Division at Sematech, reviewed the materials-intensive innovations in semiconductor manufacturing technology that have allowed the semiconductor industry to pursue both high performance and low power in logic and memory-device scaling. Recent trends show that coming up with effective ways to use heterogeneous materials systems, such as high-K dielectrics, will be the major reverse salient in continuing complementary metal-oxide-semiconductor (CMOS) scaling. Indeed, Intel has recently announced a 45-nanometer high-K metal-gate silicon-process technology based on the element hafnium.

If up to this point the exponential growth of computational power has been made possible by continued improvements within the microelectronics industry, the reverse dynamics are now coming to the fore. In other words, more powerful computers are being used as tools in the search for new materials to create the next generation of electronic components and systems. Sharon L. Nunes, vice president of technology at IBM, outlined that company's recent efforts to advance materials R&D using high-performance computing. The increased computing capability provides a more systematic way to integrate new materials into the complex microchip system than the traditional trial-and-error method. Furthermore, the new method will play a big role not only in integrated-circuit technology, but also more broadly in the simulation, modeling, and engineering of nanotechnology in the next decade.

Since the integrated circuit was invented in the late 1950s, the internal structure of the chip has grown increasingly complex, which made CMOS scaling along the Moore's law trajectory possible. The number of elements used in the production of leading-edge integrated circuits was seven before the 1990s and has increased to fifteen since then. Undoubtedly more elements will make their way into the complex silicon structure in the near future, a process in which the chemical industry will play a critical role. However, new materials innovations in semiconductor manufacturing technology will require more energy consumption, create more pollution, and introduce materials that will be much more difficult to disintegrate when discarded. Participants in this session expressed hope that computational materials science might provide answers to these problems rather than a singular focus on the miniaturization trajectory.

EMERGING GLOBAL ECONOMIES

Moderator: *Arthur Daemmrich (Harvard Business School)*
Speakers: *Theresa Kotanchek (The Dow Chemical Company)*
David Greenley (Rohm and Haas Company)

The chemical and molecular-science industries have never been confined to a single geographical area. Whether searching for raw materials and customers or low-cost labor and high-technology talent, companies have expanded beyond their home base into other areas around the globe since the beginning of the industry in the mid-19th century. In recent years the rise of Brazil, Russia, India, and China has led to increasing competitive pressure for the U.S. chemical industry and substantially reinforced the trend toward globalization. Locating R&D facilities in these emerging economies, particularly in China and India, is in vogue.

What were the forces that drove this phenomenon? Recruiting talented technical personnel—who are available in large numbers in China and India at a fraction of U.S. salaries, to be sure—is only a partial answer to this question. There are other benefits of "going local" with R&D. Theresa Kotanchek, R&D technology director at the Dow Chemical Company, and David Greenley, global director of technology operations at Rohm and Haas Company, shared their experiences in operating R&D in Shanghai, China, and Bangalore, India, among other places.

Apart from the availability of technical talent and low cost of construction and operation, locating R&D facilities in Asia allows the chemical companies to tailor products for local needs; learn about the emerging trend in the subsequent product cycle; substantially decrease turnaround time; gain closer access to customers that might otherwise be inaccessible; and learn how to do business differently within a disparate cultural context, which might feed back into the company's global operation procedures. Moreover local universities in China and India have been producing excellent research results in recent years, some surpassing the quality of work being done in the United States. Having R&D facilities closer to these newly rising centers of technical excellence will provide opportunities for the chemical industry to tap into this new reservoir of cutting-edge research.

Nevertheless potential pitfalls exist. One challenge is to successfully integrate the overall R&D effort within companies. Communication becomes a critical issue, since global teams are usually not as effective as co-located teams. Companies have experimented with advanced communications technologies, such as Web-based project tools, electronic laboratory notebooks, and video teleconferencing. On the one hand, effective utilization of information technology can mitigate some of the friction involved in the diversified site of innovation. On the other hand, different intellectual property regimes in Asia can hinder the ability to import and export new innovations. In recent years the intellectual-property situation in China has been greatly improving, especially as China itself is becoming more innovative. Differences in culture matter as well. It is sometimes necessary to provide employees with training in cultural understanding to ease some of the potential friction.

Having a global R&D footprint brings new challenges to the management and dissemination of knowledge. As the horizon expands rapidly, companies in the chemical and molecular-science industries are beginning to realize that a simple horizontal expansion or "outsourcing" of work will not suffice. Rather, successful expansion of R&D requires an organic integration of U.S. and foreign talent, accessing and creating newly rising centers of technical excellence around the world, collaborating with local industry and universities, making efforts to attract foreign investment, and connecting the global network of R&D on a 24/7 time schedule. From this perspective, the chemical and molecular-science industry is only beginning to transform itself into a truly global enterprise.

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About Innovation Day

To promote early career innovation, the Chemical Heritage Foundation and the Society of Chemical Industry jointly organize an annual Innovation Day, consisting of the Warren G. Schlinger Symposium, Gordon E. Moore Medal presentation, and Perkin Medal award ceremony. The Schlinger Symposium brings together promising young scientists and technology leaders from across the chemical industries with a focus on frontiers of chemical R&D. Plenary and breakout sessions are oriented to areas where the chemical industry interfaces with other emerging business sectors. In combination with the award ceremonies, the Schlinger Symposium offers attendees the opportunity to learn about cutting-edge science and technology, exchange ideas with peer industrial researchers and entrepreneurs, and prepare to be innovation leaders.

About the Chemical Heritage Foundation

The Chemical Heritage Foundation (CHF) serves the community of the chemical and molecular sciences, and the wider public, by treasuring the past, educating the present, and inspiring the future. CHF maintains a world-class collection of materials that document the history and heritage of the chemical and molecular sciences, technologies, and industries; encourages research in CHF collections; and carries out a program of outreach and interpretation in order to advance an understanding of the role of the chemical and molecular sciences, technologies, and industries in shaping society.

About CHF's Center for Contemporary History and Policy

The Center for Contemporary History and Policy offers historically grounded perspectives on issues related to the molecular sciences and technologies. The center's programmatic initiatives draw on diverse historical and contemporary source materials to provide knowledge, perspective, and advice to stakeholders from industry, academia, government, and citizen groups.

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