Research Frontiers
FOR THE CHEMICAL INDUSTRY

report on

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

INNOVATION DAY 09

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15 SEPTEMBER 2009

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Innovation Frontiers in Industrial Chemistry

A Report on the Sixth Annual CHF-SCI Innovation Day 15 September 2009

INTRODUCTION

Now in its sixth year, the CHF-SCI Innovation Day and Warren G. Schlinger Symposium has become widely known in the industrial-chemistry research community. It regularly draws an audience of young researchers who are seen as the future leaders of their companies' research programs. The principal objective of Innovation Day is to exchange viewpoints and to examine the broad technical issues facing the industry rather than to discuss scientific and technical details. The day also allows for recognition of achievement with the awarding of the Gordon E. Moore Medal.

Innovation Day seeks to expose its attendees 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 and of the work being done in other organizations is increasingly critical for success. We encourage participants to step back from their day-to-day operations to see the bigger picture and to network with their peers.

This report is intended to communicate conference findings to the broader audience unable to attend the event and to provide a sense of continuity with past and future Innovation Day events.

Frontier Areas for Industrial Chemistry

At the core of Innovation Day are the informal presentations and conversations that occur during the breakout workshops. Topics are selected by the Innovation Day Steering Committee, members of which secure speakers and lead the discussions.

In 2009 the breakout sessions covered the following topics:

1. Chemistry of Energy Sources
2. Sustainable Chemistry and Engineering
3. Electronic Materials
4. Emerging Global Economies

In accordance with our desire to encourage open dialogue and keep conversations "off the record," each summary in this report conveys a sense of what took place but does not reproduce the presentations. However, we do have an archive of many of the Powerpoint presentations used by breakout speakers. If you are interested in any of these, please contact rreynolds@chemheritage.org.

CHEMISTRY OF ENERGY SOURCES

Moderator: *Thomas Upton (ExxonMobil Chemical Company)*
Speakers: *Michael H. Levy (American Chemistry Council)*
Clifford C. Walters (ExxonMobil Research and Engineering)
Ellen B. Stechel (Sandia National Laboratories)
M. Stanley Whittingham (State University of New York at Binghamton)

At past Innovation Day events the cost, availability, and environmental impact of energy sources have consistently been identified as key drivers of future chemical research. Discussion of future energy sources continues to be a popular breakout topic for attendees.

Michael Levy focused his presentation on the interest of the Plastics Division of the American Chemistry Council (ACC) in "waste-to-energy" programs and their relationship to the reuse of plastics. Levy first outlined the Environmental Protection Agency's recommended waste-reduction mechanisms. Overall reduction of waste output is considered to be the highest priority, along with ensuring that recyclable materials are in fact recycled. Current recycling programs are not able to handle certain classes of plastics, a fact that led to the Plastics Division's interest in waste-to-energy programs.

Before waste ends its life in landfills, it has the opportunity to become part of the energy infrastructure of the United States. There are roughly eighty-seven facilities in the United States that convert forty million metric tons of waste into usable energy. The waste-to-energy program reduces the volume of waste by close to 90 percent. Many of the technological barriers, such as emissions, that hindered the environmentally safe conversion of waste to energy have been overcome. Further, waste-to-energy facilities provide another level of sorting that increases the amount of recyclable material (like metals and plastics) that can be reclaimed. The ACC Plastics Division sees these programs not only as beneficial in their own right but also as a means to increase the reclamation of plastics.

The group discussed the general logistics of moving waste to and extracting materials in waste-to-energy facilities, public perceptions of plastics compared with paper products (life-cycle studies show that plastic packaging materials are less environmentally detrimental than many paper products), and the investments required to obtain "energy" from waste systems.

Costs are higher than for traditional coal-fired plants but show a significant advantage when it comes to environmental impact.

Clifford Walters, while examining the chemical history of oil, characterized oil chemists as falling into two groups: those who work to find oil (exploratory chemists) and those who study how to use it (refinery chemists). Walters feels that the world will be using oil as one of its primary fuels for the foreseeable future, and believes exploratory chemists will play a prominent role in locating oil around the globe and possibly in developing scientific techniques to extract oil from living organisms in a continuous process.

Exploratory chemists have been using analytical chemistry in combination with new technologies to create a new field of study, the forensics of oil, to determine which organisms have made which types of oil throughout history. By using petroleum biomarkers these researchers are determining the history of certain classes of oil, which allows them to speculate about possible locations of undiscovered oil reserves. Walters focused on the history of certain oil compounds, detailing the science that led to the discovery of their biological precursors.

The group discussed the use of this sort of information to facilitate the production of fuels from biomass, the ability to extract oil from organisms (the challenge is to get the organism to give up the oil without killing it), and the biogenic generation of oils.

Ellen Stechel presented early-stage work done by Sandia Laboratories in the use of solar energy to create liquid hydrocarbons. While most solar technology is currently focused on the conversion of solar energy into electrical or mechanical energy, Stechel and her collaborators are interested in ways to harness solar energy to drive chemical reactions that would produce liquid hydrocarbons. Such an approach would allow many energy consumers to continue using their current processes, equipment, and infrastructure. The technological centerpiece of Stechel's presentation was a solar tower that uses energy generated by solar-energy collectors (parabolic dishes) to drive a high-temperature reaction that splits carbon dioxide and reacts with some of the products with hydrogen (derived from electrolysis of water, which can also be solar driven) to create the rudimentary alcohols.

While other technologies for creating liquid hydrocarbons exist, Stechel and her collaborators find their thermochemical process most promising given its relatively high efficiency rate. Using a solar tower with a chemical reactor that employs rotating rings to minimize the thermal decomposition of the reacting chemicals, liquid hydrocarbons can be produced continuously at a high rate. Though the technology is not yet in operation, Stechel believes that it can be a viable solution to the American need for liquid fuels.

The breakout group discussed the efficiency of the unit and source of carbon-dioxide feed. A source such as a power plant seems most likely. Reactor scale-up issues were also addressed.

The final discussion topic was M. Stanley Whittingham's analysis of the limitations of battery technologies and batteries' role in the transportation economy. He now believes that the United States is definitely moving away from the fossil-fuel era into the electric era. But implementation of this move, especially as it relates to transportation, holds a number of challenges. Not only does a new energy infrastructure have to be developed; new technologies, on both commercial and individual levels, for storing energy will also be needed. Focusing on battery-storage technologies for personal vehicles, Whittingham gave a brief overview of the technology components: electrolytes, anodes, cathodes, layered materials, and separators. He then discussed the current challenges in battery research and provided some examples of the benefits and limits of specific types of batteries. The main issue for innovators is dealing with energy density, which is hindered by the limited space of batteries in products. Currently, the use of lithium aggravates the problem, since pure lithium is difficult not only to control but also to keep compact in the storage system. A number of researchers are experimenting with the use of alternative metals, such as tin, aluminum, and silicon, to create a better supportive structure for lithium. Early results indicate that carbon skeletons with organic solvents provide an efficient medium for lithium. Nanomaterials are often hard to pack (requiring increased battery size), and, though they increase the rate for chemical reactions, such acceleration is unselective. New materials science may well be the key to overcoming contemporary problems.

The group discussed the technical specifications of various battery systems, applications for lead-acid batteries, cathodic material cost, and available additives that addressed the lithium-transport problem. Finally, the subject of electrochemical capacitors as an alternative to batteries was debated.

SUSTAINABLE CHEMISTRY AND ENGINEERING

Moderator: *Jody Roberts (Center for Contemporary History and Policy, Chemical Heritage Foundation)*
Speakers: *Julie Zimmerman (Yale University)*
Topher Buck (GreenBlue)

During the last few decades *sustainability* and *green chemistry* have become household terms. However, the terms have been used without due specificity. But what do they mean, and how will these very general visions actually be realized? Past breakout groups have tried to add more specificity. Last year's group discussed the possibility of establishing accurate and reliable green metrics on the assumption that it is only real if you can measure it.

Product and process design were the major themes in this year's "Sustainable Chemistry" session. The take-home message was that researchers, managers, and designers must all support real change for the paradigm that currently dominates design in order to achieve sustainable innovation in the chemical industry. Engineers, chemists, and industry must shift from narrow definitions of research to systemwide thinking to tackle their problems.

Julie Zimmerman began with a question: "Can we appropriately and successfully address sustainability challenges if our designs to get there are not inherently sustainable?" While she suggested that there is current, useful work that addresses such sustainability challenges as increasing cost of energy, lack of potable water, population growth, and food production, she also challenged the audience to ask themselves whether they were tackling these in a comprehensive manner that provides long-term solutions. She cited corn ethanol as a timely illustration: corn ethanol was one solution to energy challenges, but the solution created other problems, such as land-use challenges, water-quality issues rising from pesticide overuse, and the amount of carbon emitted in biofuel production. She asked whether this solution could be "the right thing, the wrong way?" Other examples of problematic solutions were given, such as the use of persistent pesticides to increase agricultural efficiency, and energy-saving bulbs, which are based on toxic metals; all are the right solutions in terms of sustainability, but were the solutions designed the best way? Zimmerman proposed that scientists and engineers who worked on these solutions may be working with good intentions, wanting to improve quality of life and work toward modernization or perhaps simply finding the science and technology exciting; but unfortunately these approaches pick one sustainability challenge to tackle, while all the other challenges, especially the ones engendered by the new design, are not addressed.

Zimmerman argued that sustainability issues, which she defined as environment plus human health plus social well-being, must be incorporated into the traditional performance equation (see Box 1).

BOX 1. A Sustainable Design Equation

Performance = function + cost + quality + safety
+ sustainability issues (environment + human health + social well-being)

She challenged audience members to think about not only how they design but also what they are designing for. Traditional design often involves incremental improvement rather than re-engineering the entire system. For example, in the car industry, designers can either try to make relatively incremental improvements in efficiency or re-engineer the whole system toward hybrid-electric or electric vehicles. Or by redefining the problem they can increase the degree of freedom in design or innovation. The car problem is not simply building a more fuel-efficient car; it is a mobility and an access challenge. Designers need to ask themselves why people get another car, what goods and services they need, and, ultimately, whether the car is the best way to deliver those things. She called for stepping back and defining the problem at the broadest scale possible. In so doing, she argued, we can actually realize the most benefits in terms of sustainability. In other words, pursue service-oriented design. What is needed to achieve this? Product and process designers need to think about the challenges they are trying to solve rather than the design they wish to make.

Topher Buck followed Zimmerman's more conceptual presentation with concrete examples. He described efforts from his nonprofit organization GreenBlue to create resources and tools to promote sustainability in the private sector. The company focuses on the designs of products, including packaging and cleaning products. Its goal is to guide companies into thinking more "sustainably." According to Buck, thinking more sustainably is both "highly contextual" and requires thinking "way upstream" at the design level.

GreenBlue believes early identification of appropriate metrics is a key to ensuring that prototypes integrate consideration of broader systemic effects. In other words, there must be some basis for judging that new prototypes are better or more likely to have fewer negative consequences, as companies or designers move toward their goal. Buck emphasized that companies and designers must look beyond equations based only on cost and performance and add sustainability, which will in turn increase the number of attributes that must be satisfied. Buck drove home the idea that systemic, long-term, and complex thinking and approaches are needed in sustainable design. GreenBlue's projects emphasize such systemic approaches. Its Sustainable Packaging Coalition brings together members that represent the whole supply chain of the packaging industry—from those dealing with raw materials, to packaging designers, to retailers—and involves them in working to define and promote a sustainable packaging industry. Further, CleanGredients is a database available to all in the industry for developing sustainable cleaning products.

Participants formed small groups to discuss sustainable designing in their particular industries. They focused on two questions:

- What drives design in your industry?
- What are the obstacles to sustainable design?

The following observations were reported back to the entire group:

- The primary driver for sustainable paint production is regulation, but the main obstacles are consumers' acceptance and the lack of industry investment in state-of-the-art R&D.

- A main driver is often cost reduction or increasing netback, and the main obstacles are economics, energy, and education.

- More general education of consumers, industry, researchers, engineers, media, and policy makers about sustainability is needed.

- Across industry and even in academia there is a need for more multidisciplinary approaches.

- The industry needs more broad company support as well as government support, including incentives to make true costs visible and, more generally, to increase appreciation for the intellectual challenge of creating sustainable design and to change the overall mind-set in the larger world. More sophisticated understanding and more complex conversations are needed all-around.

ELECTRONIC MATERIALS

Moderator: *David C. Brock (Center for Contemporary History and Policy, Chemical Heritage Foundation)*
Speakers: *Jane Frommer (IBM Almaden Research Center)*
Mike Nelson (Nanoink, Inc.)

Breakout groups in past years have shared ideas on "the next big step" in semiconductor manufacturing beyond the traditional silicon complementary metal-oxide scaling, the backbone of the last forty years of advances. That theme continued with this year's session on materials at the intersection of novel chemistries, silicon technology, and nanotechnology in advanced research on electronics. The seminal importance of the atomic force microscope as both an instrument of measurement and a tool for manipulation at the scale below 100 nanometers was stressed, and both presenters highlighted the implications and applications of atomic force microscopy (AFM) and connected technologies. There is tremendous activity at the leading edge of electronics and nanotechnology research combining novel chemistries with silicon-fabrication technology and AFM approaches.

Jane Frommer, a chemist and leading researcher in AFM, detailed three examples of this intersection. First, she reviewed IBM Research's efforts to develop their "Millipore" technology as a possible replacement for compact-flash semiconductor memory. The major advantage of Millipore technology over compact flash is its potential storage density, which far surpasses that of compact flash by some two terabytes per square inch. The Millipore technology is based on the creation of arrays of AFM cantilever tips, formed through silicon photolithography, over a highly designed polymer. The array of probes both read and write bits of data by sensing or creating small divots in the surface of the polymer. IBM's Millipore effort is an example of the use of conventional silicon approaches as a platform from which to create a new, hybrid technology that is intended to rival, if not displace, the products of this very same platform. It is an example of using today's technology to create its possible replacement.

Frommer next discussed the use of block copolymer chemistries as a means to create both "nanopores" and "nanospheres." These small structures are formed by applying various chemistries to block copolymer systems, creating matrices of the polymeric material, and then processing the matrices to add materials and remove certain other materials. By using such approaches researchers have been able to deposit highly engineered materials on silicon substrates with desirable electronic properties and to form other engineered materials on silicon substrates that are intended for applications outside of electronics, in such areas as the life sciences.

Finally, Frommer revealed very recent work conducted at IBM in collaboration with a number of academic laboratories: researchers are using DNA chemistries with silicon and AFM technology to pursue new, nanoscale electronic devices. DNA is chemically processed to form so-called DNA origami, triangularly shaped clusters of DNA. These DNA triangles are then functionalized in various ways, for example, by incorporating gold clusters or carbon nanotubes. Subsequently, the triangles are able to self-arrange into particular geometric forms on templates formed by photolithography on silicon substrates. Here researchers use DNA chemistry, one of the most studied of chemical systems, in combination with AFM and silicon technologies to find potentially extremely miniaturized electronic devices and circuits. These structures may provide a possible successor technology for traditional silicon microelectronics.

Mike Nelson, the vice president of engineering at Nanoink, Inc., discussed yet another intersection of AFM and silicon technologies with novel chemistry. Nanoink's work is directed at the commercialization of a new platform for nanotechnology broadly rather than for any single application area like electronics. Nelson's firm was started in 2001 to develop instrumentation for performing so-called dip-pen lithography. In this approach AFM cantilevers, and arrays thereof, are used to deliver various "inks" to substrates; in this way they construct nanoscale structures on a substrate. The tips of the cantilevers pick up various substances out of reservoirs and can deliver them to particular locations on the substrate. Nanoink is currently commercializing instruments for performing dip-pen lithography and pursuing applications of the platform. Potential applications include fabricating nanoscale electronic devices, but they may also be useful for such life-science applications as creating arrays for DNA and proteomics research and for the growth and development of stem cells.

EMERGING GLOBAL ECONOMIES

Moderator: *James Alder (Celanese Chemical)*
Speakers: *Cong Cao (The Levin Institute, The State University of New York)*
Marc E. Kalton (Edica-Garnett Partners, LLC)

Globalization and the rapid growth of such emerging economies as China and India present dramatic prospects for expansion and diversification into new markets as well as new sites of innovation. As chemical companies seek to take advantage of this growth, they must also address such issues as industry consolidation, changing supply-chain patterns, regulatory compliance, and environmental concerns that may require different approaches in each regional setting. For the third consecutive year the presenters focused on China and India because of the size and scope of activities in these two countries.

Cong Cao made a convincing argument for the likelihood that China will be successful in achieving a state of "indigenous innovation" by 2020; he also argued that China will achieve first-class status in the world by 2050 through its strong science and technology innovation capabilities. As supporting evidence he presented data on the sharply rising trajectory of Chinese-authored science and technology papers, which show increasing levels of sophistication; a significant expansion in higher education; and increasing R&D investments (including foreign direct investments), all drawing on a very large talent pool. Cao specifically highlighted the following areas of emphasis in the growth of Chinese innovation:

- applied research based on societal needs (agriculture and manufacturing, energy, environment, transportation, public health, national defense, and public security);
- frontier technologies (biotechnology, information technology, lasers, new materials, aerospace and aeronautics, and ocean, energy, and manufacturing technologies);
- mega-science projects (protein science, quantum research, nanotechnology, and developmental and reproductive biology); and
- mega-engineering projects (semiconductor manufacturing, broadband wireless mobile communication, nuclear power, water-pollution treatment, AIDS and hepatitis treatments, aircraft manufacturing, and space exploration).

Steven Freilich reviewed with the audience the experience of DuPont in achieving business success in China. He noted that the megatrends of today are dominated by the emerging economies, which in turn are dominated by China and India. According to Freilich, when entering an emerging economy, building market access is the first order of business. As an aside, he also noted that DuPont received its first order from China in 1863—interestingly, for gunpowder—and he recounted the history of China's significance in the nineteenth-century world marketplace.

Returning to the theme of local market development, he pointed out that DuPont first re-entered China in 1975 and through a careful process of nurturing people and markets now has six thousand employees in China and investments of over $100 million. To respond appropriately to the competition that is now both global and local, a multinational company like DuPont has to develop locally in each country. In the final analysis being able to attract and retain the best people in each situation is the critical success factor.

Marc Kalton presented his perspectives on the growth dynamics of R&D in China and India with the catchphrase "you can't not be there." Through a series of comparisons both between the two countries and with the rest of the world, Kalton made his case that the cultural and economic drivers are producing significant needs and opportunities. Specifically, he pointed out that China is now a major world R&D player whose spending will soon surpass Japan's, while India is just awakening.

Kalton then presented a specific list of needs, opportunities, threats, and challenges faced by all who are attempting to engage in these countries. He made the point that success requires managing the process—on the macro level by understanding corporate objectives, establishing methodical plans, and organizing for success, and on the micro level by critically managing "life on the ground." To illustrate the concepts Kalton then presented success stories for Danfoss, Wyeth, Pfizer, GE, Lanxess, and Honeywell. He finished his remarks with the summary observation that both countries are "can-do" societies and that both realize we are all in a competitive global village.

APPENDIX I: CASE HISTORIES OF INNOVATION IN MATERIALS SCIENCE

Continuing a practice that was initiated last year, an optional workshop was held for those arriving early on the afternoon before Innovation Day. "Understanding the Dynamics of Materials Innovation" was based on two recent case studies completed by CHF's Center for Contemporary History and Policy.

The Robert W. Gore Studies in Materials Innovation examine the dynamic process of conception, development, manufacturing, marketing, and regulation of new materials innovations in the contemporary world. In building source collections, case studies based on in-depth research focus on a particular materials innovation, making explicit the lessons for researchers, research managers, and policy makers. Despite the importance of new materials in economic growth and social change, we understand little about the process of materials innovation. Studies are meant to help governments better prepare for economic and social changes, allow industry leaders to organize better for successful innovation, give universities tools to better link to industry, and offer insights to the public and nongovernmental organizations.

David Brock reviewed his study on the rise of chemically amplified photoresists for manufacturing semiconductor microcircuits. In the early 1980s researchers realized that the then-dominant process on which semiconductor manufacturing technology was built—photoresist—would soon be insufficient if the pace of miniaturization were to be maintained. Therefore, a radically new form of photoresist would be required. This case study examined the innovation of the first of these radical "chemically amplified photoresists" by IBM in the 1980s.

Four findings have implications for our understanding of the nature of innovation. First, the case points to the critical role of diverse individuals who bring aspects of their background experience to bear in a constant process of partial transfer. These partial transfers were then hybridized to yield novel developments. Second, the case demonstrates the process by which researchers' intentions and materials are mutually reshaped through intensive interaction. This interplay gives rise to new knowledge. Third, the case revealed the centrality of what Brock termed *imagined economies.* Researchers' beliefs about economic factors profoundly shaped their decision making, even preceding inventive activity. Fourth, the case shows the systemic nature of materials innovation: that is, innovation occurs in an ecosystem of existing technologies. The innovation process for chemically amplified photoresists was bounded by an existing structure in this technological ecosystem, most particularly lithography exposure tools.

Chris Magee, co-director of engineering design and advanced manufacturing at the Massachusetts Institute of Technology, reviewed his work on quantifying the role of materials innovation in overall technological development. Magee has been studying rates of technological progress in various fields and what factors drive the innovation. The first issue is what metric can reliably measure the rate of development. He suggested a number of functional performance metrics that have been used for various industries. These metrics should measure progress over a significant period, for example, fifty to seventy-five years.

In looking across a wide variety of fields Magee has shown that rates of progress are remarkably constant over long periods and are characteristic of the field. For instance, the growth rate of battery capacity was 3 percent per year, while improvement in the rate of information transport was 35 percent. The group discussed the implications of these observations and which metrics might appropriately measure technical progress in their industries. One interesting observation was that progress in capacitor development was outpacing that in battery development, a factor that should be considered for the field of energy storage.

Magee concluded with some general observations: materials-process innovation contributes at least 20 percent of the progress in all areas examined; the contribution of materials-process innovations in the field of energy storage are possibly 80 percent or higher; and the relative contribution of materials-process innovation to overall technological progress has grown in the last few decades.