**Report of a Workshop on New Mechanisms for Support Of High-Risk and Unconventional Research in Chemistry**

Submitted to the National Science Foundation
July 21, 2003

Submitted on behalf of the Participants by:
Ralph G. Nuzzo and George M. Whitesides (co-Chairmen)

r-nuzzo@uiuc.edu
gwhitesides@gmwgroup.harvard.edu

**DISCLAIMER**

The workshop described in this report was supported by the National Science Foundation under Grant No. CHE-0333251. Any opinions, findings, or conclusions are those of the authors and do not necessarily reflect the views of the National Science Foundation.

## EXECUTIVE SUMMARY

A group of academic scientists and engineers met at the NSF in Arlington on May 17-18, 2003 to discuss mechanisms for funding "high-risk" and unconventional research. Specifically, this group considered whether it would be desirable for NSF to develop an experimental program designed to support highly innovative research (which might be high-risk, in areas relatively unfamiliar to chemistry, or unconventional in focus or structure of the programs); that is, research of types that would be difficult or impossible to support by existing NSF programs. One of the many tasks assigned NSF by the federal government is to foster and support world-leading fundamental research. There is a broad concern that NSF has been increasingly inhibited in this task by limited resources, and by the characteristics (both strengths and weaknesses) of the peer-review system.

The underlying motivation of this discussion was to advise NSF in new mechanisms to make it possible for chemists to address "big" problems and problems considered too risky to be acceptable to the peer review process as currently practiced, and if required by these problems, to carry out research involving resources—both human and financial— on scales not available under existing programs and with current procedures.

The committee concluded that there were, in fact, a number of opportunities for NSF to do business in a way that would make it both more responsive to unconventional ideas, and more proactive in helping the community to develop and shape new ideas. It developed—as a hypothesis for NSF to consider—the concept of a program that would support Centers (either real or virtual), having a number of key features:

- *A Focus on a Big Problem, and a Common Vision.*
- *Three to Six Highly Talented Investigators and a Strong Leader.*
- *Representation from a Range of Skills and Approaches.*
- *A Critical Mass in Financial and Human Resources.*
- *Local Autonomy with accountability, in Allocation of Resources, in Personnel, and in Direction.*
- *A Culture of Innovation and Risk-Taking.*

As an exercise, and to focus its thinking, the committee developed a model for the Centers. In this model, the Centers would be developed by the investigators in active cooperation with NSF using a phased approach, and be organized to emphasize ambition in their choice of problem, focused and committed teamwork by highly skilled investigators, a collaborative and multidisciplinary style, and an administrative structure designed to promote innovation.

A key part of the proposal was a staged program in developing a proposal. In this proposal, a concept would move from initial formulation to final proposal in a series of steps—each having a gateway that used peer review—following a process designed to encourage team-building, extensive planning, and proof-of-concept experiments, all supported by NSF in appropriately structured, sequential sub-programs.

**RATIONALE.** Chemistry is at the center of the sciences. It has been the most reductionist of the sciences that is concerned with perceptible reality; it is a rich source of useful technology; it is the bridge between physics, biology, and materials science. It is also replete with important, unsolved problems: the molecular origin and basis of life; the nature of materials; the nature of chemical bonds; the properties of individual molecules; the characteristics of the liquid phase and its influence on molecular reactivity; and the properties of molecular assemblies. These subjects, and many more, provide examples.

Despite its central position among the sciences, and despite its rich set of opportunities, Chemistry has a reputation that falls short of matching its high intrinsic excitement and value. It is seen (by the public, by the government, and most importantly, often, by chemists!) as a mature discipline that works on important but highly specific problems: that is, as a field important to chemists but not widely understandable and interesting to the larger society. It is also perceived as a field whose intellectual agenda is often set based on its industrial applications. The system of support for chemistry, and the structure of chemistry departments in universities, have been important in its development of these characteristics. It has become a prototypical "small science" field: chemistry is largely carried out by individual investigators, working with relatively small groups, on problems that often are based on current professional interests in chemistry, rather than on larger problems in science and society. Collaborations involving chemists, although growing in importance, still do not begin to cover the range of opportunities open to collaborative research. The peer review system—with its characteristic preference for high-quality, familiar science—dominates the process of allocating resources. The successes of chemistry seldom attract public attention. It has become a field that tends to favor development over risk taking.

The question posed to the committee was "Is there a structure for the organization and support of chemistry that would favor more audacious and ambitious research, would encourage the expansion of chemistry into new areas, and would develop new ways for chemists to operate, both among themselves and with scientists in other fields?" The objective of a new structure would not be to replace the existing structures and associated processes (which, on the whole, operate well). Rather, it would be to accelerate the rate of invention in chemistry, by providing an opportunity for especially able and ambitious groups of investigators—sharing a commitment to a "big problem"—to pursue these problems in a program designed to have a high administrative tolerance for risk.

The committee was asked to consider if there were administrative experiments that the NSF might sponsor and support that would help chemistry to be more adventurous. The mission of NSF is to encourage and support the best research: are there new procedures it could use to fulfill its mission?

The committee concluded that there were, in fact, a number of opportunities for NSF to do business in a new way. It developed—as a *hypothesis* for NSF to consider—the concept of a program that would support *Centers* (either real or virtual), having six key features:

- ***Focus on a Big Problem, and a Common Vision.*** The Centers would join small groups of investigators to work, with their students, on a *big* problem: that is a problem with the potential for major impact on science and fundamental understanding, and with major visibility in society.

- ***Highly Talented Investigators.*** The success of these enterprises—as in any scientific enterprise—would depend on the people that they engaged. This program would be designed to make it possible to recruit the best possible people to work on the problems that were the foci of the Centers.

- ***A Range of Skills and Approaches.*** The Centers would enable research that would be impossible to do in the context of a single research group. To do so, they would almost certainly be constituted to include a range of skills (within chemistry and from adjacent disciplines) and approaches (fundamental, applied, theoretical, and experimental).

- ***A Critical Mass.*** The Centers would provide a level of support to the major participating groups that would be large enough to be a major part of the income of the group, and thus, the focus of loyalty and effort. It would also involve enough people and enough talent to provide a critical intellectual mass, even in new and difficult problems.

- ***Local Autonomy and Agility.*** The NSF would delegate authority to the Centers to make decisions that would enable them to optimize their performance in real time, without time-consuming oversight.

- ***A Culture of Innovation and Risk-Taking.*** The NSF would explicitly expect the Centers to be innovative and audacious, and would accept a concomitant risk of failure higher than the peer review system might normally accept in NSF's standard programs.

**OBJECTIVE AND DESIGN OF THE PROGRAM.** The committee, and the chemical community, supports the central, continuing value of peer reviewed, single-investigator grants, and acknowledges (in fact, emphasizes!) that many of the best ideas in chemistry (and more broadly, in science) have come from such programs. The intersection of small research groups and the peer review process tends, however, to lead to the selection of familiar problems, and problems that have a high probability of succeeding, and does not provide reliable methods for evaluating and supporting unconventional, unfamiliar, and high-risk ideas. There are also problems that may require, to be successful, a structure that is significantly different from the type of grant commonly awarded by NSF in chemistry—that is, problems that are significantly different from the norm in size, in resources required, in skills that must be engaged, in the type of evaluation used, or in management: among these problems are those that require the combined skills of a number of different investigators and disciplines.

**RECOMMENDATION:** The committee concluded and recommends that NSF should *experiment* with an alternative structure based on multiple investigators focused on a single, shared problem, working in a Center (or distributed research team) designed to allow groups of particularly able and particularly committed investigators to work on unconventional or high-risk projects that could not be handled by existing mechanisms of support. The major difference between this Center concept and other NSF programs would be the way in which the focus and participants of the Center would be developed. This process would be designed to make it possible to *develop* the team, concept, and initial proofs of concept required to justify a major investment by NSF in unconventional research, while staying within the constraints of the peer review process. This process is outlined below.

The ***objectives*** of the Centers would be:

***To Make It Possible for Chemistry and Chemists to Take On Large Problems.*** Chemistry is now a small science: it does not have programs like the human genome project or nanotechnology, nor does it make much use of large facilities such as the Hubble telescope or a major synchrotron light source. The fact that it chooses to work primarily with small, single-investigator grants fits much of the work in the field, but doing so makes it difficult for chemists to work on projects that *are* sufficiently ambitious that numbers of different skills (and thus, of people) are required for rapid progress. It also excludes chemistry from some of the most important current problems in science and technology.

***To Make Chemistry More Visible.*** The small research projects favored by chemistry also have the characteristic that they are largely invisible outside of the profession. Synthetic methods, or methods of simulation, or the details of mechanisms are all intensely interesting to chemists, but difficult for non-chemists to understand. As a consequence, successful chemical research seldom appears in the popular press, and chemistry is not a science whose excitement and benefits are visible. Unfortunately, some of its failures—especially environmental pollution—*are* visible. The field needs a mechanism to allow it to undertake projects that are sufficiently big, adventurous, audacious, unconventional, and risky that they *do* attract attention, and that they *do* have the potential to change how people think about the world. It can not and should not be a primary objective of academic research to attract favorable public attention, but some such attention attracts students and resources, and provides protection from the inevitable failures.

***To Foster New Areas of Chemical Inquiry.*** Chemistry tends to focus on a small number of themes at a time. One consequence of this focus is an over-emphasis on the fashionable fields, and an under-emphasis on exploration of *new* fields. Chemistry would benefit from a mechanism of support that would allow the establishment of new areas of research. Single-investigator programs can only support a subset of the possible opportunities.

***To Build New Communities.*** To have a field of science flourish, it must be based on a community of scientists and engineers with common interests. This community provides stimulation, satisfies the need for peers for review, provides an audience for new work, allows its members to compete for funds, and exchanges ideas and students. Evolving a new community based solely on small, single-investigator grants is a slow (10-20 years) process; larger programs (for example, DARPA programs), if properly constituted, can build a community more rapidly (that is, over a period of 3-5 years). DARPA programs are, *per se*, probably not appropriate for NSF for a variety of reasons, but larger programs centered on a common theme could have the advantage of creating a community.

***To Put Researchers with Common and Complementary Interests Into Productive Contact.*** Some of the most productive areas (and areas with the *highest* probability of producing new results) are often those that catalyze the interactions of groups of investigators working across the boundaries of disciplines. Examples are materials chemistry, chemical biology, and environmental chemistry. Larger programs can encourage these types of programs, and chemistry would benefit from increased interactions among different areas of chemistry, and among areas of science.

***To Develop New Methods of Engaging the Interest in the Public.*** A multi-investigator program has the resources and the range of talents to innovate in the development of mechanisms for engaging the public. Whatever the focus—working with schools, teachers, or museums; developing teaching materials; writing popular books—requires time and interest. Some individuals have that interest; some do not. The committee expects that a Center would normally have as part of its staff someone with the time and interest to lead such efforts, with the resources to implement them, and with the explicit responsibility for doing so. A multi-investigator group centered on a topic having public appeal clearly has an important opportunity and obligation to engage the public in its work—to the benefit of the public, that area of research, and chemistry as a whole.

***To Develop a Shared Culture of Risk-taking and Innovation.*** Chemistry is perceived as being conservative and averse to risk. It needs mechanisms of support that have as an *explicit* part of their objective the development of communities of researchers who are, and are encouraged to be, exploratory, and willing to undertake important but risky projects. The existence of a program having risk-taking in the name of the major innovation would help to encourage the chemical community to think about innovative but risky problems.

**WHAT ARE EXAMPLES OF "BIG PROBLEMS"?** An objective of the program would be to allow chemists to take on "big problems". What *are* "big problems"? Simply to clarify its collective thinking, the committee suggested several topics as having the potential to form a productive focus for multidisciplinary groups, and to engage public attention. This list is *purely* for illustration: the chemical community would have to propose its own projects and visions. Since NSF-supported research relevant to these examples is already going on, the list also suggests the point that projects that already exist, in weakly interacting, dispersed form in NSF-supported research might—when aggregated—have greater visibility and be able to move more rapidly.

- **Revolutionary Materials.** The development of functional materials with genuinely unexpected functional properties (to take two current examples, high $T_c$ superconducting materials, and materials with negative index of refraction) has the potential for great impact in both science and applications. Effective programs in this area typically require the combined efforts of investigators interested in synthesis, properties, measurement, theory/simulation, and applications.

- **Origin of Life.** Chemistry and biology have been making slow but steady progress toward understanding how living systems might have begun. Now might be the time to start a coordinated, multitalented attack on this problem.

- **Bonding.** Bonds determine the properties and structures of matter. An initiative to understand chemical bonds better, and to encourage the design and discovery of new types of bonds, could have major impacts on our fundamental understanding of chemistry and of new materials, medicines, and the environment.

- **Molecular Assemblies.** Chemistry has a far better understanding of molecules than of *assemblies* of molecules (both structures and dynamics). Molecular aggregates are fundamental to molecular recognition in biology (and, thus, the rational design of drugs), to the structure of complex structures in the cell (and thus to life), and to materials science (and thus to polymers and other materials crucial to a technological society).

- **Water.** Many of the most important chemical transformations in living systems and in the environment occur in water. Water is ubiquitous in its importance: it is the solvent of life; it is the stuff of oceans and a major component of the atmosphere, and thus a major part of the environment. It is also at the core of increasing levels of international conflict. Its properties and influence on dissolved molecules, and on reactions among those molecules, is remarkably incompletely understood. And *everyone* understands that water is important.

- **Ultimate Chemical Analysis.** Chemistry has made remarkable progress in extending analysis to the level of single molecules and atoms. Single molecule spectroscopy, scanning probe methods, and other instrumental techniques have opened to door to the examination of the properties of single molecules. The development of yet more advanced tools has the potential to change chemistry's understanding of "chemical reactivity", to help to understand the normal and diseased cell, and to contribute to national security.

**STRUCTURE OF THE CENTERS**

The committee considered a number of different types of organization. The one selected combines an emphasis on the excellence of individual researchers with a structure designed to make it possible to tackle difficult but important problems. This section sketches the structure that seems best to meet the need for collective research activities focused on ambitious, unarguably important, visible, and risky research. This structure is, again, *one* possibility, and other structures might fit other needs or different types of problems that the NSF might wish to encourage the community to attack.

- ***The Core: A Shared Vision.*** The key requirement for the type of program envisioned in this recommendation—and for the type of commitment that would be required by NSF—is a shared vision of a large scientific problem, an area of research, and of an approach to it. Without this vision, the program would never cohere, and would become something like other programs ("glue" grants; MRSECs; others). These programs are unquestionably good ones, but there is no need to replicate in a new program what they already offer.

- ***Leadership.*** A Center requires leadership. The natural tendency for successful science is fractal growth. An objective of this type of program would be to have all parties—the principal investigators, the participants, the NSF—agree on a theme and a focus, and then to stick with it until it was proved successful and reached maturity, or proved a failure and was terminated. The leadership of the Center should, ideally, ultimately rest in a single individual (or few individuals), rather than in a democratic executive committee. Idiosyncratic, intense, focused vision is not typically the product of a committee.

- ***Active Involvement by NSF.*** To make a Center with ambitious objectives successful will require *active* involvement from all participating parties, *including* NSF. The NSF style has been to remain primarily administrative. The administrative role is, of course, essential, but—as other agencies, especially DARPA, have demonstrated—it can be very helpful for the sponsoring organization (in the form of an active, imaginative, and committed program manager) to play an active role in an ambitious, complicated, multi-Center research program. NSF could help manage connections between research groups, provide opportunities for public involvement, work to ease communications, collect relevant information from the scientific community, offer friendly, informed criticism, stimulate the Center to solve difficult problems or to move on, and help to ease the administrative burden so that the Center director could spend his/her limited time in doing science, not accounting and report writing. NSF should make sure that an engaged, entrepreneurial program manager has *personal* responsibility for, and active interest in, a Center.

- ***Virtual or Collocation.*** The committee did not make a recommendation about the relative value of Centers that were *real* (that is, located in a single university) or *virtual* (distributed across several universities). As a practical matter, most Centers would probably be virtual. An objective of a Center would be to bring together the best possible set of principal investigators. The leadership of a Center should be free to recruit countrywide and (with restrictions on the types of expenditures that could be made and activities supported) *worldwide*. Although there are certainly advantages to co-location of the participating research groups in a single university, in fact it is improbable that the best investigators in a single area would be in a single place: universities tend explicitly to build departments based on diversity of interests, rather than on concentration. The Centers should thus assume that participants would be geographically scattered, and make an active part of the program the full and imaginative use of all forms of communication (and especially of cyber tools, since they offer probably the newest opportunity to change the way science is done). In particular, the budget for a Center should include funds for videoconferencing, for desk-to-desk, low-resolution video cam communication among students, for the support of shared electronic workspaces, and for virtual manipulation of expensive, shared instrumentation. The programs should also assume that they would use travel, technology and exchange of students, as important ways of building a genuinely committed and functional scientific enterprise with shared goals, tools, and information, and the expenses for this kind of communication should be an explicit part of the budget for the Center.

- ***Scale.*** The appropriate scale of the project would depend on the problem selected for its focus, on the research program proposed, and on the availability of participating groups. The committee suggests that a scale of three to six university research groups would be manageable, with a sufficient amount of money to each that the project becomes a significant (ideally largest) source of support (probably $300 –400 K per year) for that group. As the programs of a funded Center evolve, so may the types of supporting infrastructure that are required: the instrumentation, plant, and supporting services.

- ***Participation.*** The participants should be selected to include the groups best qualified to attack the problem. In general, these groups would be academic research groups in the U.S., but if some of the best talent were in industry, government laboratories, or outside the U.S., the NSF should be able to find a way of allowing their inclusion at some level. The key issue is that the NSF should find ways of allowing the group to include the best possible participants, rather than posing administrative difficulties hindering it in doing so. Since the subjects that form the foci of Centers will often include matters relevant to a number of disciplines, it is probable that the Center teams will be multidisciplinary (although centered in chemistry). Industrial participation should be allowed, if it provides expertise needed by the Center.

- ***Uniqueness.*** An important criterion for the Center is that it take as its mission a problem and approach that could not be handled by existing programs.

- ***Program Development.*** NSF must use peer review to judge the quality of the proposal ultimately submitted. Peer review—correctly—could not and would not approve $2 –3 MM/year for an unproved idea. The committee suggests a process consisting of a series of stages—supported by NSF, but at levels starting with inexpensive planning workshops, and leading through graded stages in increasing effort and financial support to the final proposal and Center—that would allow the team to form, refine its goals, demonstrate its effectiveness, and generate proof of concept for important ideas. This progression (discussed in greater detail in the section entitled "Proposal") would eliminate some of the risks (especially risk in the degree of commitment of the team to its area of focus, and in its organizational and scientific effectiveness) in the proposal, and make it practical to have it reviewed by peers.

- ***Integration of Disciplines and Approaches.*** It is often true in modern science that some of the most exciting work is done at the boundaries between disciplines. Including in the group a broad range of approaches, disciplines, and skills should be an integral part of the design of a Center, and one in which NSF may be able to help. Although the Centers should be focused in Chemistry, they should certainly have the flexibility to include participants from other areas of science, and from engineering, if it is needed to achieve the objectives of the Center.

## PROCESS FOR DEVELOPING A CENTER

Selecting and supporting Centers of the type suggested here poses a problem for NSF, because it mixes two apparently incompatible elements.

1. **A Focus on Highly Innovative, High-Risk Research.** The objective of a Center would be to carry out research on areas that had *not* been subjected to extensive previous research—areas in which the members of the Center believed that there was a potential—even a high probability—of a major scientific success, but in which there might be little initial work, and no established peer community.

2. **A Requirement for Peer Review.** NSF operates by peer review. Peer review normally works best in evaluating projects that are "normal" science: that is, science that fits in a context of on-going work, and in which there *is* a peer community qualified to judge proposals.

So, the conundrum is: "How to use peer review to evaluate a proposal in a high-risk area when there is no peer community and when peer review does not work well in new, high-risk projects?" The committee did not have a complete solution for this problem, but suggested a staged process. The development of a Center would not be one in which a "win or lose" proposal was submitted and reviewed, but rather a process proceeding through a number of steps: an initial, short white paper; development of the idea and the team through workshops and meetings; low-level funding to establish proof of principle, and to demonstrate the ability of the team to work together; full funding. *Each* of these steps would be separately peer reviewed in some way, with the initial stages being rapid (and generating small amounts of funding), and the last steps being rigorous and leading to full funding of the Center. NSF would be expected to play a helpful role throughout this process, rather than to be only a reviewing/funding/administrative body. **Overall, forming a Center would involve a multi-step *process* involving several stages of review and increasing levels of funding, rather than a single *proposal*.**

***Development and Funding Processes***. The committee envisioned the proposal as proceeding through six stages. Each of these stages should provide a level of evaluative discrimination for NSF, and of useful feedback to the group forming the Center.

1. **Idea**—the definition of a big problem, and the conception of an initiative in research that would lead to major advances in chemistry by an (the) investigator(s).

2. **White Paper**—The presentation of a refined program concept, schematic model for the work to be carried out, and suggestions of a proposed group of initiating participants in the form of a formal White Paper, and its evaluation by the NSF. By keeping the white paper (and its review) short, NSF could encourage groups of investigators to explore their best ideas, and could engage imaginative, and busy, members of the community in their review. Successful submission and review of a white paper would generate funds to use for workshops and meetings to discuss and refine the idea and to plan initial experiments.

3. **Planning Stage**—the development of a more fully developed plan based on the invitation of the NSF and recruitment of the members of the Center via a formal planning process. This developmental stage could include support from the NSF for Workshops, Conferences, and Travel as might be appropriate for developing the materials for a formal pre-proposal.

4. **Pre-Proposal**—a formal evaluative document that would be subject to peer review. The pre-proposal would outline the program goals and the

plan of work that would serve as the foundations of an initial program. It would allow comment by NSF (and perhaps by peer consultants) on strengths and weaknesses of the concept, team, and proposed program. It would contain significant information, but not so much as to be a major effort to write. Successful review of the pre-proposal would result in an invitation by NSF to submit a full proposal. The understanding would be that a program that had reached this point would have a significant chance (perhaps 1/3) in being funded.

5. **Proposal**—a full proposal describing a program, broken into two phases. The first phase would focus on demonstration of concept. Funding of this phase would give a subset of the investigators modest levels of support to demonstrate key proofs of concept. The second phase would include the goals for the full Center, and an outline of benchmarks which, when achieved, would trigger full funding to achieve these goals. This proposal would again be subjected to peer review.

6. **Staged Growth to Full Funding Based on Accomplishments and Milestones**—the final stage of the process of developing a full Center: the stage at which initial-phase programs reaching their term would either terminate or compete via a full proposal process for funding as a Center**.** The understanding would be that a successful completion of the initial phase of research—where "successful" implies both technical success in proof-of-concept research, and management success in building an effective team—when combined with an excellent proposal based on those successes, would have a *high* probability of being funded.

In the latter stages of this model, the committee is suggesting a process that roughly follows the philosophy of an SBIR program. The initial program serves as a point of entry, but is not as expensive (in dollars for NSF or in time spent writing proposals for the investigators) as a full proposal. The planning process and the white paper are also critical elements. The committee believes it is important to allow small planning grants to be awarded after a successful completion of a white paper stage to facilitate the construction of the proposal for the initial stage of the research.

The committee suggested that the programs that compete successfully in the initial phase should be funded at a level of approximately $500 K per year and run for a term not to exceed three years. The programs at this stage would involve the likely collaborative interactions of groups of three or four senior investigators. Proposals that successfully compete at the subsequent stage would enter into a phase of staged growth that would raise them—consistent with the requirements of maintaining suitable progress and realization of the programs goals and requirements—to the funding level of a full Center. The committee believes these Centers should receive funding that allows the program goals to be met, builds the specialized infrastructure and other resources needed to support the research, and allows the addition of senior investigators as needed.

Each case should be argued separately as to the funding levels that would be appropriate, but sums of the order of $2.0 to 3.0 million per year for programs running for a term of five years would be reasonable. It is essential that the budget explicitly include administrative support, and funding for a specialist in outreach. If the Center director is being asked to accomplish something extraordinary in research, it is not practical for him/her also to carry the high administrative burden that typically goes along with being the head of an NSF center.

## *REVIEW CRITERIA AND PROCESS OF REVIEW*

***Review Criteria and Process of Review.*** Centers, and the earlier programs that would precede them, would be subject to several cycles of review and evaluation. The procedures followed to evaluate these proposals would differ in some regards from those followed for the types of grants typically awarded by the Chemistry Division of the NSF. The evaluations in every case would, nonetheless, center on a set of essential metrics--ones considered in the context of, but in addition to, the two larger evaluative criteria required of all awards made by the NSF. Evaluation would require that four requirements be addressed. The Center should demonstrate that it had (or would have, when fully formed):

1. *A Big Problem.*
2. *A Multitalented, Multidisciplinary, and Multistyled Team.*
3. *A Requirement For Existence Establishing that Other Programs Can Not Support It*
4. *Proof of Concept of Its Central Ideas.*

Determining that a proposed Center met these requirements would require special care on the part of NSF. First, reviewers must be carefully instructed by the NSF staff to take into account the special characteristics of the program, and especially its emphasis on big, unconventional, and/or high-risk problems. These might be used to select white papers and pre-proposals that would advance either for further development or more formal review. The committee fully endorses the use of screening committees, site visits, and reverse site visits at appropriate stages. The final selection of Centers for full funding should be based on a combination of mail and panel reviews.

It is anticipated that the 5-year Center projects would be reviewed in mid-course by NSF staff with panel/visitor assistance, and then re-reviewed for a second 5-year funding duration near the end of the $4^{th}$ year of the project by the mail/panel review process outlined above.

***THE ROLE OF NSF***

**In Developing the Centers.** The committee believes the NSF should play a central role in developing these Centers. The historical role of NSF has been administrative. There are, however, very imaginative program managers in NSF—individuals with broad exposure to science and a strong sense of what constitutes important research—and these individuals are not fully used in their current, largely administrative, roles. The committee suggested that the NSF consider a role in which it worked with groups *actively* during the development of a Center. The leadership of a Center must, of course, come from the investigators, but help from NSF personnel could increase the probability of success of good projects (and, incidentally, provide a challenge and a source of satisfaction for the program manager).

**In Advertising the Program, and the Purpose of the Centers**. With a new program, one of the difficulties is, of course, to inform the community of its existence, to convince that community that the program is a serious, new effort, and to persuade the community that it is worth the time and effort to become involved and to compete for support under it. If NSF chooses to proceed with this experiment, it will have to make a serious effort to expose the concept of the Centers to academic chemistry. It will also have to explain the unfamiliar process for developing a Center, and explain that this development process provides an increasing probability of success, as the effort in going forward with each stage increases.

**In Operating and Managing Funded Centers.** Every aspect of the program will have to be built from scratch, since there is no history of this kind of Center or process. It would be a crushing burden, in the view of the committee, were the full weight of developing the processes needed to manage these Centers to fall entirely on the first few programs. It is essential that, while maintaining exceptionally high standards and demands for the scholarship produced in the program, that the NSF and the members of the Centers should build effective lines of communication. They both share with the community a deep interest in the success of the Centers.

**In Outreach.** Outreach is another central area where the NSF and Centers must work together cooperatively. Again, the committee strongly urges the NSF to adopt requirements in this area that do not place heavy administrative burdens on the awardees. Similarly, the Centers should be active and imaginative in their outreach (especially since increasing public awareness of chemistry is one of their basic justifications). The NSF can be an effective partner in outreach and public awareness, and also should include in the support of the Centers funds to pay for an individual who is a specialist in outreach.

### *METRICS FOR PERFORMANCE AND SUCCESS*

The Centers should be judged on the basis of six criteria:

1. *First-class research focused on a big problem.*
2. *Results that could not be obtained by a single investigator.*
3. *Achievement of demonstrable milestones agreed on by negotiations with NSF.*
4. *Integration: horizontal (across disciplines) and vertical (from fundamental to applied)—using an architecture agreed on in discussions with NSF.*
5. *Active and productive interaction with the public.*
6. *A culture of innovation: science, education, and social impact.*

### *DURATION AND RENEWAL*

The lifetime of the grant will depend on the nature of the program proposed. The initial stages of a program should be funded for terms of a maximum of three years, and should be ineligible for renewal. Funding for full Centers should be for 5 years, with extension for another 5 years based on excellent performance in the first cycle. Renewal for a second 5-year period would require submission of a grant application that would be reviewed competitively with others.

## SUMMARY CONCLUSIONS AND RECOMMENDATIONS

The committee concluded that there was an opportunity and an obligation for NSF to develop new methods of supporting exciting new ideas in chemistry. The need for new mechanisms is particularly acute when the ideas are at the border of chemistry and other fields, or focused in "big" problems in a style uncharacteristic of chemistry, or concerned with areas or styles of research that are currently not fashionable or in which there are no well-established peer communities.

The committee suggests, as a hypothesis for NSF to consider, the concept of *Centers* bringing together multiple investigators to work on new, big, high-risk areas.

NSF would play an active and important role in developing these Centers to the point that they would pass the scrutiny of the peer review system by staging support: from low levels for planning and recruiting the team, thorough intermediate levels for demonstrating proof of principle and building the team, to full operation.

These Centers could also serve as laboratories for new techniques for carrying out and managing research in chemistry. The extensive use of information technology (to facilitate interactions among the participants) and of techniques of outreach (to build public awareness of Chemistry) are particularly interesting areas for exploration.

## APPENDIX I: MEMBERS OF THE COMMITTEE

**CBC Workshop Participant Contact List**

John I. Brauman
Stanford University
650-723-3023
brauman@stanford.edu

Ralph G. Nuzzo
University of Illinois at Urbana-Champaign
217-333-1370
r-nuzzo@uiuc.edu

C. Grant Willson
University of Texas at Austin
512-471-4342
willson@che.utexas.edu

Larry Dalton
University of Washington
206-543-1686
dalton@chem.washington.edu

Jillian Buriak
Purdue University
765-494-5302
buriak@purdue.edu

MG Finn
The Scripps Research Institute
858-784-8845
mgfinn@scripps.edu

William L. Jorgensen
Yale University
203-432-6288
william.jorgensen@yale.edu

George M. Whitesides
Harvard University
617-495-9430
gwhitesides@gmwgroup.harvard.edu

Paul A. Wender
Stanford University
650-723-0208
wenderp@stanford.edu

Anna C. Balazs
University Of Pittsburgh
412-648-9250
balazs1@engrng.pitt.edu

Tobin J. Marks
Northwestern University
847-491-5658
t-marks@northwestern.edu

Laura L. Kiessling
University of Wisconsin-Madison
608-262-0541
kiessling@chem.wisc.edu

Joanna Aizenberg
Bell Laboratories, Lucent Technologies
908-582-3584
jaizenberg@lucent.com

Luis Echegoyen
Clemson University
864-656-5017
luis@clemson.edu

Matthew D. Shair
Harvard University
617-496-4591
shair@chemistry.harvard.edu

Alejandra Palermo
Royal Society of Chemistry
44-020-7440-3333
ap206@cam.ac.uk

## APPENDIX II: CHARGE TO THE COMMITTEE AND TERMS OF REFERENCE.

**The objective of this workshop (May 17-18, 2003) is to ask if there are new ways in which the Chemistry Division of the NSF might invest some of its funds on an experimental basis to help to introduce new opportunities into chemistry, to make research centered in chemistry more visible and more exciting (both to scientists and to society), and to strengthen the most innovative part of academic chemistry.**

The hypothesis underlying the workshop is this:

Now is an exceptionally interesting time for chemistry: it has built an enormously powerful and sophisticated base in its core areas, and it faces a range of exciting problems both in the core and in new areas. Despite this happy circumstance, it also has structural problems: much of what chemistry does is invisible (and incomprehensible) to the public (and often to other areas of science and engineering); it is organized (within the Chemistry Division at the NSF) almost exclusively around small, single-investigator grants, and thus restricted to the kinds of research that can be done with those grants; it conducts relatively little of its research in cooperative efforts, and thus benefits only slowly from the lateral spread of new ideas; it is often perceived to be a mature science that is focused on technical issues. It seems possible that structures other than single-investigator grants might allow chemistry to expand its horizons and its influence.

We would like to address four questions in this workshop:

**1. Are there big problems in natural science that fall naturally and centrally within the scope of chemistry as a discipline, that have the characteristic that they would be understandable and exciting to chemists, to other scientists and engineers, and to society**

**as a whole, and that might benefit from complementary research by a number of research groups (certainly inside chemistry, but also in adjacent fields)?**

> *Examples* of problems (chosen purely to give a sense for a scale that seems reasonable for the workshop to discuss) that might fit these criteria are "The Origin of Life" and "Science to Accelerate the Development of Developing Economies".

**2. Are there structures for supporting research in these areas that might be considered as alternatives to isolated, single-investigator grants?**

> *Examples* of such structures might be localized centers, delocalized/virtual centers or collaboratives, and programs actively connecting networks of individual investigators through periodic meetings, exchange of students, and travel.

**3. If NSF were to try an experiment in non-traditional organization of research in chemistry, what would be appropriate mechanisms for peer review? NSF uses "intellectual merit" and "broader impact" as criteria in its review process: how should these phrases be applied and interpreted in experimental programs that might develop from these discussions? How would one tell if an experiment were a success?**

> *Examples* of important considerations in the peer review process include the structure of the review groups (choices include those already used--*ad hoc* panels, site visits, reverse site visits, mail review...-- but also might require a new structure); the vectors used in measuring success (scientific excellence, technological importance, education, training, societal importance, nucleation of change within the chemical community, influence on policy and public awareness, ...); the composition of the programs (the quality of the investigators, industrial involvement, international participation, ....); and others.

**4. Should the Chemistry Division of NSF consider one or two experiments in non-conventional modes of support, and if so, what should these experiments be?**

We would ask you to come prepared to offer your opinions, specific suggestions, and wisdom about these questions. Please develop an initial set of talking points that can be presented to the other participants of the workshop in the form of a (single) summary overhead slide.

The *product* of the workshop will be a short, written report (which will be largely finished by the end of the workshop) answering the four core questions.

George Whitesides

Ralph Nuzzo

## APPENDIX III: Proposal.

## Proposal for a Workshop Entitled:
## "Chemical Bonding Centers: New Organizations to Address Emerging Areas of Opportunity in the Chemical Sciences"

## I. Project Summary

The contributions made by chemistry are felt throughout society. With a traditional focus centered on a core set of molecular scale problems—structure, reactivity, synthesis, mechanism, catalysis, tools for molecular biology, theory, methods of analysis, biochemistry—the knowledge engendered by chemical research has transformed essentially every area of modern technology. These advances have come from research efforts organized according to a number of models—ones relevant to the varying needs of the diverse group of public and private sector entities active in the field. Universities historically have adopted a model built on collections of individual programs—ones involving grants awarded to a single senior investigator—as a means of fostering progress in research. Programs involving collaborative interactions between several senior investigators have been less common in the past, but more recently have come to play a larger role. The considerable progress made in the core areas of chemistry research speak to the success of this system.

Chemistry is experiencing a level of change that is unprecedented in its history. It is finding applications for molecular science that fall far outside the areas that have defined its past. These emerging areas of opportunity develop challenges and may require methods of address unlike that encountered in the past.

This proposal requests support from the National Science Foundation for a workshop involving participants who largely hold faculty positions in research intensive universities. The focus of the workshop will be on the roles that could be served and benefits derived from the establishment of Centers that would bring together large teams of investigators to attack the new frontier challenges in chemistry. The workshop, organized by Ralph G. Nuzzo (the University of Illinois at Urbana-Champaign) and George M. Whitesides (Harvard University), will develop materials needed to construct a report that will be delivered to the Chemistry Division of the National Science Foundation. The meeting will be held at the NSF Headquarters Building in Arlington Virginia on May 17$^{th}$ and 18$^{th}$, 2003. Funds are requested to support the travel and per diem expenditures of the participants and cover the administrative costs of the organizers.