INSTITUTE FOR DEFENSE ANALYSES

An Evaluation of the National Security Science and Engineering Faculty Fellows Program

Stuart A. Wolf
James Belanich
Melissa A. Cummings

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INSTITUTE FOR DEFENSE ANALYSES
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For More Information

James Belanich, Project Leader
jbelanic@ida.org, 703-845-6606

Leonard J. Buckley, Director, Science and Technology Division
lbuckley@ida.org, 703-578-2800

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Executive Summary

Background

The Department of Defense (DoD) established the National Security Science and Engineering Faculty Fellowships (NSSEFF) program in 2008 to support distinguished university faculty and staff scientists and engineers who are conducting potentially high pay-off basic research on topics of interest to DoD. In 2016, the name of the program was formally changed to the Vannevar Bush Faculty Fellowship (VBFF) to commemorate Dr. Vannevar Bush's role in directing and elevating DoD research and pioneering research by the U.S. Government.

The VBFF program is directed by the Basic Research Office of the Assistant Secretary of Defense for Research and Engineering, who asked the Institute for Defense Analyses (IDA) to review the VBFF program, provide a program overview, describe accomplishments of the research efforts made possible through VBFF funding, and make recommendations for the continued success of the program.

Methods

A mixed-method approach was used in this review. First, phone interviews were conducted with awardees from the first 3 years of awards and with the founder of the fellowship program. Next, a literature review was conducted for publications on research findings supported, at least in part, by the fellowship. Additional analysis was conducted to determine indicators of research impact, which included identification of peer acknowledgement through membership in professional societies and bibliometric analysis. Finally, the IDA team attended a meeting of what is planned to be an annual meeting between DoD laboratory personnel and fellows.

Findings

- *The VBFF program has had a significant and positive effect both on the development of new scientific directions made possible by the size and longevity of these awards and on the Principal Investigators'* (*PIs*) *careers.* The level and length of funding enabled the fellows to explore innovative ideas, which frequently paid off, and to build critical mass in new domains, while most other research grants would not allow for such growth and progress. It was also noted that the minimal oversight burden and the flexibility given to the PIs enabled

them to steer their research in directions that would have been impossible under typical award conditions.

- *Most of the fellows in the first three classes have been recognized for their excellence by their peers in numerous ways.* Twelve are members of one of the three national academies and four more have provided advice to one or more of the national academies. Eighteen of the awardees have achieved the distinction of being elected fellows in their respective professional societies. Twenty-three have received at least one merit-based award from their respective professional societies or associations.

- *This program has evolved significantly over the last decade.* The first two classes were exposed to a novel selection process that included an interview process that the awardees really liked. Several scientists even felt that this was one of the most significant events in their lives. The 2010 class was selected by a more traditional process (i.e., white paper, down-select, proposal, review, and final selection). From 2011 to 2013, there was a 3-year hiatus in selecting new awardees. This was due mainly to the transfer of this program from the Basic Science Office of OSD to the STEM Development Office, where their priorities were understandably different. Despite there being no new awards during this period, the original three classes were funded for the full 5 years. In 2014, the program was moved to the Basic Research Office at the urging of its Director, Dr. Robin Staffin. The program was resurrected, and new awards were made starting in 2014, with additional awards in 2015, 2016, and 2017 under the management of Dr. Aura Gimm and Dr. Jiwei Lu, with direction from Dr. Staffin.

- *Interviewees from the initial three classes noted a lack of an organized interaction with DoD scientists and/or laboratories.* Even though many academics had an established relationship with the DoD or became involved as a result of this fellowship, others were disappointed that they did not have a formal opportunity to interact with DoD scientists and felt that this was one weakness in the program. Annual meetings were held in 2009 and 2010, but they were discontinued when the program was redirected into STEM efforts. Annual meetings held at various Service labs were reinstated in 2014, and have continued. Also, in 2016 a pilot program, the Laboratory University Collaboration Initiative (LUCI), was started to promote collaboration between DoD researchers and research fellows. LUCI funds DoD Laboratory scientists to work in collaboration with the fellows, enabling DoD researchers to leverage the research being conducted through VBFF.

Research Accomplishments

Summaries of the research accomplishments from all of the fellows from the 2008–2010 classes are included in Appendix A of this report. Some of the accomplishment highlights that NSSEFF enabled include the following:

- New methods for growing semiconductors crucial for high-performance optical components.
- Producing nanopillars with increased precision for use in advanced computing and communication technology.
- Designed new proteins with enhanced antiviral properties.
- Developed auditory testing technique to assess cognitive processing problems.
- Developed innovative process for producing piezoelectric greatly increase energy harvesting properties.
- Developed new computer model for hypersonic flows.
- Built novel DNA circuits that can be used for medical diagnostics.

Recommendations

- To keep the award prestigious and highly competitive, maintain funding for approximately 50 concurrent fellows (i.e., 10 new awards each year).
- To promote exploration and flexible research to make significant breakthroughs, continue to allow the fellows to adjust research plans as they progress.
- To maintain attractiveness of fellowship, maintain high level of funding and only high-level oversight (low burden).
- To leverage research capabilities developed through the fellowship, develop alumni group that maintains ongoing links to DoD laboratory research and scientists.
- To leverage skills gained by graduate students and post-doctoral researchers, explore methods for increasing their participation in future DoD research efforts (e.g., working for DoD, applying for future DoD research grants, working for DoD contractors).
- To expand dissemination of research advancements, increase efforts to promote research findings to industries crucial to DoD.
- To maintain technical expertise in the selection of fellows, leverage academic and industry expertise for proposal review process and consider a return to a distinguished panel of experts for final review.

Contents

1. Introduction

The Department of Defense (DoD) established the National Security Science and Engineering Faculty Fellowships (NSSEFF) program in 2008 to support distinguished university faculty and staff scientists and engineers conducting potentially high pay-off basic research on topics of interest to DoD. In 2016, the name of the program was formally changed to the Vannevar Bush Faculty Fellowship (VBFF) to commemorate Dr. Vannevar Bush's role in directing and elevating DoD research and pioneering research by the U.S. Government. In addition to conducting innovative, "blue sky" research, an additional goal of the VBFF program is to foster active, long-term, well informed research programs in areas of interest to DoD that will attract and develop creative and energetic scientists, engineers, and their students. The VBFF program also encourages relationships between the program's fellows and DoD science and technology personnel.

The VBFF program is directed by the Basic Research Office of the Assistant Secretary of Defense for Research and Engineering, who asked the Institute for Defense Analyses (IDA) to review the VBFF program, provide a program overview, describe accomplishments of the research efforts made possible through VBFF funding, and make recommendations for the continued success of the program.

A. Historical Background and Program Evolution

This program was initiated in 2008 by Dr. Will Rees, who was the Deputy Undersecretary of Defense for Laboratories and Basic Sciences. His goal was to build an ongoing program with a steady state of 50 awards (i.e., approximately 10 new awards per year, each award for 5 years) (Rees 2015). He wanted to augment the model for traditional DoD funding for basic research and provide a significant grant for distinguished scientists to explore science domains that are important to DoD. Rees' intention was that the NSSEFF would have a prestige along the lines of the National Institutes of Health Pioneer Awards and the National Science Foundation Waterman Award.

This program evolved significantly over three periods in the past decade:

- Period 1. Initiation of NSSEFF Program (2008–2010)
  - First 2 years, all scientific disciplines eligible
    - Funding at $600,000/year for 5 years
    - Awardees required to have received PhD less than 25 years ago

        - White paper review by Government STs[1]
        - Finalists interviewed by panel of DoD and Government officials
        - Final selection made by Rees
        - Requirement for DoD clearance (Secret)
        - Yearly program reviews with DoD scientists
    - Third year all scientific disciplines eligible
        - Dr. Rees no longer with DoD
        - Funding ceiling increased to $850,000/year for 5 years
        - "Not meant to be an early career award"
        - No panel interview, more standard evaluation of proposals by Government and DoD experts
        - Final selection made by Dr. Andre von Tilborg, Deputy Under Secretary of Defense for Science and Technology, and IDA
        - No clearances required
- Period 2: Program Hibernation (2011–2013)
    - Program moved into newly formed OSD STEM Development Office
        - No new awards made but existing awards were continued with little or no oversight by or connection to DoD labs
        - No technical leadership in STEM Development Office to manage program
        - Funds reallocated to educational purposes
        - Staffin-Wax report recommends moving program back into Basic Research Office from Education
        - Basic Research Office held workshop in June 2013 to review progress of NSSEFF projects and published a report including research summaries (Gimm, 2013)
- Period 3: Resurrection and Institutionalization of Program (2014 to present)
    - Program moved into Basic Science Program Element

[1] ST is a government position classification for a senior-level research and development position. It is at the Senior Executive Service level, but instead of directing an agency, STs are conducting high-level research.

- Dr. Aura Gimm and Dr. Robin Staffin reinstitute the awards in 2014
- Dr. Jiwei Lu takes over Dr. Gimm's role in 2015
- Not an early career award
- List of suggested topics with relevance to DoD areas of interest, but all scientific disciplines are eligible
- Funding reduced to $600,000/year for 5 years, allowing for more awards in 2014
- White paper and full proposal paper review by Government experts (full proposals are reviewed by academic and industrial experts)
- Final decision made by Dr. Robin Staffin, Director for Basic Research
- Name of program is changed to the Vannevar Bush Faculty Fellowship
- Laboratory University Collaboration Initiative (LUCI) pilot program initiated to promote connections between fellows and DoD Labs

The NSSEFF program was renamed the Vannevar Bush Faculty Fellowship program in 2016, in honor of Dr. Vannevar Bush (1890–1974) to honor his influence on the development of the U.S. military research enterprise. Bush served as the director of the U.S. War Department's Office of Scientific Research and Development during World War II. Before the war, Dr. Bush was a professor and dean of engineering at the Massachusetts Institute of Technology, and he founded an electronics company that grew to become the defense contractor Raytheon. As a basic researcher, Bush developed some devices that enabled the development of computers. In 1945 Bush authored a report titled *The Endless Frontier,* where he recommended an expansion of government support for basic science and the establishment of the National Research Foundation, which became the National Science Foundation. Bush outlined five principles to effectively foster support for scientific research: (1) stability of funds over years to sustain long-range programs, (2) agency oversight by individuals with understanding of scientific research, (3) use of grants or contracts to fund research, (4) independence of universities and research institutes for specifics of conducting research, and (5) only high-level oversight of research efforts.

The DoD defines (Department of Defense Instruction 3210.1) "basic research" as the

> systematic study directed toward greater knowledge or understanding of the fundamental aspects of phenomena and of observable facts without specific applications towards processes or products in mind. It includes all scientific study and experimentation directed toward increasing fundamental knowledge and understanding in those fields of the physical, engineering, environmental, and life sciences related to long-term national security needs. It is farsighted high payoff research that provides the basis for technological progress.

The DoD invests in basic research to develop and exploit new knowledge and create innovative future capabilities, and it uses multiple programs and initiatives to accomplish this. This varied approach is a strength of DoD basic research since it adapts to diverse missions and motivations to conduct research of value to national security (National Research Council, 2005). Some of the other funding mechanisms for basic research include the multidisciplinary research initiative (MURI), which funds collaborative research efforts with potential for both defense and commercial application, Service-funded single-investigator awards that focus on particular areas of military need, Defense Advanced Research Projects Agency (DARPA) awards that address high-payoff technology development, and in-house laboratory research conducted by DoD laboratory personnel. In a review by the Defense Science Board (2012, 23), the NSSEFF program was highlighted as a valuable program that contributes to DoD basic research.

B. Program Overview

The intent of the program is to fund potentially transformative research in topics areas of interest to the DoD. The expectation is that funding "bold and ambitious 'blue sky' research"[2] may subsequently alter the path of scientific disciplines or create new fields of study. In addition, the program seeks to enable the development of a scientific workforce that will work on DoD research efforts for years to come. According to the OSD Basic Research Office, the program objectives[3] are to:

- Support unclassified basic scientific and engineering research that could be the foundation for future revolutionary new capabilities for DoD
- Foster long-term relationships between university researchers and the DoD
- Educate and train student and post-doctoral researchers for the defense workforce
- Familiarize university researchers and their students with DoD's current and projected future challenges
- Increase the number of talented technical experts that DoD can call upon.

The fellows are selected through a competitive two-step process that evaluates the scientific and technical merit of proposals submitted by a principal investigator (PI). The first step is a three-page white-paper submission that is reviewed by subject-matter experts from DoD and other government research facilities. The top 20–30 white-paper proposals (semifinalists) are then asked to submit full proposals, which are reviewed by subject-

2 http://www.acq.osd.mil/rd/basic_research/program_info/vbff.html.

3 Ibid.

membership in and receipt of honors from professional societies was done through internet searches of the relevant organizations and databases. The determination of h-indices for fellows was completed through Scopus[4] and was based on the awardee's entire career.

To gather additional background information and perspective, the IDA team also attended a 2-day meeting (5–6 April 2016) of new awardees and DoD lab representatives at the Army Research Lab, Adelphi, MD. This meeting represented a new annual meeting process that is planned to continue in future years at different DoD research facilities around the country. Also, Will Rees, the former Deputy Under Secretary of Defense for Laboratories and Basic Sciences and the primary OSD leader who developed and initially directed the NSSEFF program in the 2008–9 time frame, was interviewed on 15 December 2015 to gain a better understanding of the initial purpose of the fellowship along with his perspective on how it has evolved since its initiation.

D. Programmatics

The NSSEFF award was authorized under U.S. Code, Title 10, Section 2358, which permits DoD to engage in basic research of potential interest to the DoD. The NSSEFF program was funded through annual appropriations through Program Element 0601110D8Z, to support "world-class researchers in scientific areas of critical importance to DoD and ensures the cultivation of exceptional talent. Fellows' work spans a broad set of emerging scientific areas with transformative potential."[5] The intention of the program is to foster connections between academia and the DoD basic research enterprise. Also, the fellows should provide DoD with deep scientific expertise from research universities and collaborate with DoD scientists and engineers.

Faculty with tenure or full time research staff who have the skills, knowledge, and resources necessary to conduct the proposed research as the principal investigator (PI) at an institution of higher education (university) with doctoral degree-granting programs are eligible to apply for this award. Applicants must be a U.S. citizen or permanent resident, and are expected to have a record of substantial scientific contributions.[6] PIs may submit only one application for a particular year's competition. Applicants from Historically Black Colleges and Universities (HBCUs) and Minority Institutions are encouraged to submit proposals. Note, however, that no portion of award will be set aside exclusively for HBCU and Minority Institution participation.

[4] Scopus, a database of peer-reviewed publications, provides a comprehensive perspective on research output (https://www.scopus.com/).

[5] The National Security Science and Engineering Faculty Fellowship (NSSEFF) program was realigned from the National Defense Education Program, Program Element (PE) 0601120D8Z, to PE 0601110D8Z for Basic Research Initiatives beginning in FY 2015.

[6] http://www.grants.gov/view-opportunity.html?oppId=284735.

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2. Findings

Through the interviews, review of publications, and analyses of research publications described in the previous sections, IDA made a variety of findings that demonstrate the impact of the NSSEFF program. These findings address how the program has changed since its inception, the research impacts and outcomes enabled by the awards, and the perspectives of both awardees and those who were semifinalists in the competition during the first few years of the program.

A. Awardees Perspective on the Program

During the interviews with 27 of the awardees from the first three award classes, IDA found that they were more than willing to provide their perspective on the program and related outcomes from the awards. Although the comments were overwhelmingly positive, interviewees provided constructive criticism as well. The comments covered proposal process, programmatic features, impact on field of science and fellow's career, contributions to DoD future workforce by providing graduates students with relevant experience, continued collaborations with DoD, and where the program didn't live up to expectations.

The interviews were focused on the research output, as is described in the summaries of each awarded fellowship in Appendix A. During the interviews, however, the fellows commented on how the program enabled those scientific outcomes and had other beneficial byproducts. Below is a summary of those secondary benefits beyond the specifics of what was discovered during the fellowship:

- A majority of the awardees described how the fellowship enabled strong advancements in their field of research.
- A majority of awardees stated that through the fellowship they created strong, ongoing relationships with DoD researchers.
- Over half stated that the fellowship was a significant boost for career advancement, leading to national recognition in their field and new professional opportunities.
- The program features mentioned most positively (by over half the awardees) was the size of the award, the minimal oversight, and its long tenure, which allowed for a broad perspective on an area of research and the ability to take calculated risks and adjust the line of research as they progressed. A third of the

awardees characterized the flexibility of the award as a key strength of the program.

- Almost 40% stated that the fellowship provided financial support to graduate students who have subsequently joined the workforce and begun contributing directly to DoD research (i.e., working for a DoD lab or acting as a PI on a DoD funded project).
- Some of the fellows cited that the fellowship helped establish spin-off companies that are advancing state-of-the-art technology development.
- Of the fellows from the first 2 years, about half mentioned a positive outcome from the panel review that extended beyond receiving the award. Of the fellows from the third year who did not have an in-person panel review, one-fifth stated that they had heard about the panel review and wished they had experienced it.

The comments during the interview were very positive about the fellowship and what it enabled the researchers to accomplish. The only weakness in this program mentioned by about one-third of the awardees was they would have liked more formal interactions with researchers from DoD labs. Starting in 2016, annual gatherings of the fellows at DoD labs have been instituted. The LUCI also started in 2016. Both these adaptations to the program should help alleviate the missed opportunities for building more robust relationships between the fellows and DoD researchers.

B. Funded Research

Appendix A contains summaries (approximately two pages each) of the research conducted by the researchers from the first three classes of fellows (29 summaries). These projects have all been completed, and there has been sufficient time to assess the initial impact of their work. As with most foundational research, the full impact of the efforts may not be known for several years. We can therefore expect that additional benefits will come from the completed research efforts. Because of the several year hiatus in making awards, the newer projects are still ongoing, and it is too early to make a valid assessment of their impact, although there will be some comments about them below. The summaries provide a qualitative description of the goals of the respective projects, their accomplishments and, where appropriate, the interactions of the fellows with DoD laboratories and scientists.

C. Indicators of Research Impact

There is no single metric of research output that fully captures the impact of an individual's contribution to science. This section addresses the scientific impact of the program as suggested by general indicators of research quality. The indicators of research quality include peer acknowledgement through honors/awards, selection by peers to professional research societies, and selection to advisory boards, as well as a rating of scientific production (i.e., h-index).

1. Peer Acknowledgment

One method to identify a quality researcher is through the perceptions of other well-regarded members of their individual research communities. All the fellows from the classes of 2008–2010 have received some type of formal acknowledgement from their peers in science for their quality of research since they received the fellowship. These indicators of quality include being nominated to be a fellow in an academic society or professional organization, being asked to advise the government or a large organization on a scientific matter, or winning an award or other competitive honor.

One of the higher honors for scientific excellence is an invitation to become a member of the National Academies of Science. There are three National Academies, one each for Science, Engineering, and Medicine. Of the 29 fellows, 7 were elected to the academy before their fellowship, indicating that they were a highly valued member of their research communities and recognized for their distinguished achievements in original research. Five fellows were elected member after they received the fellowship, indicating that their current research along with previous research was considered exemplary. Four additional fellows who had not been elected were asked to provide advice to committees of the National Academy. This level of achievement by 16 of the fellows demonstrates the high quality of the Vannevar Bush Faculty fellows.

Other science-oriented societies and organizations also bestow member/fellow status upon individuals based on their distinction in a particular field or research domain. Eighteen of the Vannevar Bush Fellows received such distinction since they began their fellowship at organizations like the American Academy of Arts and Sciences, Institute for Electrical and Electronics Engineers, Materials Research Society, Acoustical Society of America, American Institute of Chemical Engineers, American Chemical Society, and the Optical Society of America.

Most of the fellows have won additional awards for the quality of their research. Twenty-three of the 29 fellows won at least one merit-based award since they received their fellowships. These include major awards such as a Guggenheim Fellowship and a Humboldt Award (Chang), the Royal Society of Chemistry’s Centenary Prize (Mirkin), the R. W. Wood Prize of the Optical Society of America (Murnane and Halas), the Willis E. Lamb Award for Laser Science and Quantum Optics (Murnane, Halas, and Kasevich), Materials Research Society Medal (Glotzer), Frank Isakson Prize of the American Physical Society (Halas), the Von Hippel Award of the Materials Research Society and the Wolf Prize in Chemistry (Lieber), MacArthur Fellow and Lemelson-MIT Prize (Rogers), IEEE Photonics Award (Weiner), Society for Industrial and Applied Mathematics’ John Von

Neumann Lecture Prize (Greengard), and the Polymer Physics Prize of the American Physical Society (Olvera de la Cruz)

NSSEFF fellows are sought after for technical advice. The high quality of the fellows has also been recognized by organizations who have asked them to participate in some formal advisory capacity. Fifteen of the fellows have performed in an advisory role for a range of organizations and governmental agencies. These include National Science Foundation, National Research Council, National Institute of Health, President's Council of Advisors on Science and Technology, DARPA, Department of Energy, Institute for Computational and Experimental Research in Mathematics, American Association for the Advancement of Science, and Bureau of Ocean Energy Management (Department of Interior).

2. H-index

One measure of scientific impact is the h-index, which for a given researcher equals the number of papers (published journal articles), where the number of citations is greater than or equal to the number of papers (Hirsch 2005). For example, a researcher with 15 published papers, and 10 of those publications with at least 10 citations each, would have an h-index of 10. By taking into consideration the number of papers produced and the quantity of citations for each paper, the index characterizes the scientific output of a researcher in both productivity (number of papers) and significance (number of citations) into a single value. As with all indicators of scientific impact there are some limitations to the h-index, which include variability across research fields and insensitivity to some publication patterns (Alonso et al. 2009; Costas and Bordons 2007). Therefore, we will not use h-index to compare researchers to each other or across fields, but only use h-index to indicate a general level of productivity that is demonstrated by influential researchers.

According to Hirsch (2005) an h-index of approximately 12 would be typical of an academic achieving tenure, an h-index of approximately 18 would be typical for advancement to full professor, an h-index of 15 to 20 would typically indicate a fellowship in a national society, and an h-index of approximately 45 would be associated with membership in the National Academy of Sciences for the United States. For the 29 fellows from the first 3 years, the average h-index was 53.4, with a range of 17 to 134. This suggests that most of the researchers are accomplished, with even the least still at an impact level of a newly appointed full professor.

D. Changes over the Years

1. Panel presentations for the first 2 years—The initial paper review was by Government STs and the final "in person review" was an interview by a distinguished government panel. The first panel included Norm Augustine as the Chair and Brendan Godfrey (head of the Air Force Office of Scientific Research

[AFOSR]) as a panel member. Dr. Rees said that the panel "made the finalists sweat and the process was good mental practice." He envisioned that there would be an annual meeting at the secret level and a separate half-day poster session. His model fellow was Professor George Whitesides,[7] who would help the government when needed. He felt that the requirement of a clearance would help the programs linkages to the DoD as he never felt that the program should be isolated. In retrospect, he felt that the program could have done better in this respect, and this was borne out in some of the interviews with the fellows. This model was followed for the first two classes (2008 and 2009), but by 2010 the panel interview was replaced by a paper review. Section 2.E includes the perceptions of people who participated in the panel presentations but did not receive awards.

2. Pause in awards—There was an initial group of awards in 2008–10, then a suspension of new awards during 2011–2013, and then the award was reconstituted starting in 2014. During 2010–2014, budget allocations to NSSEFF were significantly reduced and fluctuated considerably from year to year. Starting with the budget for FY2015, the program was transitioned from the program element for National Defense Education Program to Basic Research Initiatives. The process has stayed consistent during 2014–2016, with the expectation that it will continue to award approximately 10 new fellowships each year.

3. Laboratory University Collaboration Initiative—LUCI is a mechanism to foster collaboration between DoD Lab researchers and the VBFF recipients. In 2016 LUCI was piloted to augment the NSSEFF program support for collaborative research projects between DoD researchers and NSSEFF fellows in areas of scientific or technological importance to DoD, while also expanding the research capabilities of DoD Labs. With LUCI, there is an internal-to-government competition whereby government laboratory researchers are provided with funds to collaborate with NSSEFF awardees.

4. Level of oversight—During different periods of the program there have been different levels of capability to provide oversight. Because of the fellowship nature of the program, intense oversight is not warranted, and might even hamper research productivity of the fellows if extensive reporting requirements

[7] Dr. Whitesides, a chemist and a professor at Harvard, has made numerous contributions to science (e.g., nanotechnology, nuclear magnetic resonance spectroscopy, and soft lithography) along with frequently advising the DoD, NASA, and NSF. He is a member of the American Academy of Arts and Sciences, the National Academy of Sciences, and the National Academy of Engineering, and he is a fellow of the American Association for the Advancement of Science and the American Philosophical Society. He has been awarded numerous patents and won several awards and honors from professional societies.

were instituted. On the other hand, having technical expertise from the Service labs and the Basic Research Office provide some oversight can help keep projects focused on research important to DoD, but a key aspect of this is the technical capability of those reviewing progress. During Period 2 of the program, when no new awards were being made, there was little technical oversight of the research because of the lack of access to experts in particular research domains in the OSD STEM Office. When the VBFF transitioned to the Basic Research Office, there was access to technical expertise that could provide meaningful technical oversight.

5. The initial two classes all had to attain secret-level clearance—The requirement that all VBFF awardees obtain a secret-level clearance was eliminated because the process to get a clearance was slow and there was no clear benefit to the program. The research proposed and conducted by the awardees occurred mostly at universities in facilities that were not set up to handle classified material, and the burden to modify research facilities did not appear to be worthwhile. Also, because the research being funded was basic research, there was an expectation that it would be published in the open literature.

E. Information from Finalists Who Did Not Receive Awards

During the interviews with awardees from the first 2 years of the Vannevar Bush Fellowship (2008 and 2009), several awardees made surprisingly strong positive statements that the panel interview process helped shape their research through the insightful questions from the panel. Several of the awardees specifically said that the panel review was "life changing" and extremely high quality. The strength of the statements was surprising, but because the evaluation team had only received the perspective of the awardees we decided to attempt gain perspective from those finalists who participated in the review panels but did not receive an award.

We emailed all 19 of the finalists in the first 2 award-years who did not receive awards with four general questions: (1) How would you describe the application process (initial white-paper stage, the full proposal stage, and the in-person panel review)? (2) Were you able to secure alternative funding for the ideas in your proposal? (3) Did the proposal process change how you viewed DoD funding? (4) Did the proposal process influence your subsequent interactions with DoD research labs? A space for additional comments was also provided. We received responses from 11 of the 19 finalists.

Regarding the application process, nine respondents felt that the process of applying for the fellowship through a white-paper submission was conducted well and was relatively standard, but three respondents stated there was some confusion to what was needed or that the process seemed disorganized. Regarding the in-person panel review, three respondents thought the process was good and the panel provided thoughtful interactions/questions, three were neutral to the process, and five considered it strange or that the membership of the panel was such that they might have difficulty understanding their proposals.

Among the finalists who didn't receive funding through the fellowship program, nine respondents stated that the found alternative funding mechanisms, while only two respondents stated that they didn't (both also said that they didn't submit similar proposals for alternative funding). The DoD organizations where alternative funding was obtained included the Office of Naval Research (ONR), AFOSR, OSD-DURIP (Defense University Research Instrumentation Program), and DARPA. Two of the respondents stated that they subsequently received private (nongovernment) funding for their research. Most of the respondents (eight) stated that not obtaining the fellowship did not change their perception of DoD funding, and they continued to pursue DoD funding as they had in the past. One respondent was inspired by the Vannevar Bush proposal/panel process and sought out new DoD funding mechanisms for their research. Only two respondents stated that they were discouraged by the process.

Five of the respondents had little prior interactions with DoD research, and three of those were inspired to work more with DoD in the future, and two stated that they didn't strive to work with DoD in the future. Six respondents had already worked with DoD, and the experience of being a finalist without winning a fellowship did not deter them from wanting to work with DoD in the future.

In the section for additional comments, several respondents indicated that they considered NSSEFF to be a good program and very prestigious fellowship. Other comments indicated a misunderstanding about topic priorities since there was a perception that only a few topic areas were supported, whereas all topic areas were open for the first three classes; others had a misconception about the possible range of funding levels that could be supported; and finally, some had a misconception about the targeted seniority of the faculty where in fact it should have been clear that applicants in the first two classes had to have received their PhD less than 25 years from the application date; the third class Funding Opportunity Announcement clearly stated that this award "was not meant to be an early career award."

3. Summary, Conclusions, and Recommendations

A. Summary

Summaries of the research accomplishments from the 2008–2010 classes of fellows along with their perceptions of the program are included in this report (see Appendix A). Excerpts from some of the summaries follow here:

- Connie Chang-Hasnain—New methods for growing III-V semiconductors (e.g. (In, Al)GaAs and In(Ga)P) on silicon substrates, crucial to enable high-performance optical components like light-emitting diodes (LEDs), lasers, and amplifiers to be grown directly on silicon complementary metal oxide semiconductor (CMOS) electronic circuits. This technique led to the first optically pumped nano-laser, a single pillar solar cell, and the first LED directly grown on silicon.
- Diana Huffaker—Precisely controlled the position, geometry, and dimension of nanopillars (NP) to form highly uniform NP arrays. Manipulating the degrees of freedom has allowed them to probe new functionalities in optoelectronic devices, such as light trapping to improve solar cell efficiency, and creating photonic crystals that may be used for advanced computing/communication technology.
- Stephen Mayo—Designed new proteins that have antiviral properties, one of which show an eighteenfold ability to neutralize HIV. This research may lead to enhanced neutralization potency against influenza.
- Carey Priebe—Research developed a unifying algorithmic framework for fusing disparate data types across different domains. This has led to advancements in neuroscience (mapping neuronal activity), detecting human trafficking (finding bad actors through social network activity), and image analysis (distinguishing change in surveillance images).
- Barbara Shinn-Cunningham—Developed a novel technique to test auditory sensation and perception to determine hearing and auditory cognition. This led to a correct understanding of cognitive processing problems of some military personnel that had been mischaracterized as hearing impairments, which will lead to more appropriate treatment options.

- Susan Trolier-McKinstry—Research produced innovative processes to produce new materials with piezoelectric properties that can enable microelectromechanical systems (MEMS) to physically control movement of very small parts, which will allow for smaller robotics systems. These new piezoelectric materials can produce a nearly tenfold increase in power generated in energy harvesting from the environment, which may enhance surveillance and sensing systems used in the battlefield.
- Graham Candler—Developed new code that changed how computers model and simulate hypersonic flows (speeds above Mach 5). The codes developed, which are now used by Air Force Labs and the Naval Air Warfare Center, are mandated by DARPA to be used by their contractors working in hypersonics.
- John Rogers—Developed innovative electronic materials that are flexible, which allows them to be used in novel ways like printing epidermal electronic systems on skin to be used as biosensors measuring brain, heart, and muscle activity.
- Andrew Ellington—Built multiple novel DNA circuits that demonstrate some of the possibilities of biological software, such as for medical diagnostics.

B. Conclusions

The VBFF is a strong basic research program supported by the DoD that has produced some significant advances in science and new technology. Continued and strong support for the VBFF will be vital to helping keep the United States at a technological advantage over its adversaries. At its current level of approximately 10 new fellows per year, this program should remain prestigious and highly competitive.

The first three classes have now completed their research and have produced some significant scientific and technological advancements:

- New methods for growing semiconductors; manipulating light in novel ways that may improve computing/communication technology.
- Designing new antiviral proteins with improved ability to fight HIV and other viruses.
- Developing new algorithms for fusing disparate data.
- Developing a novel techniques for accurately determining hearing/cognitive impairments in warfighters exposed to blast injuries.
- Producing new piezoelectric microelectromechanical systems that can be used in extremely small robots or for harvesting energy.
- Creating new code for accurately simulating hypersonic flows being used by DoD for developing hypersonic vehicles.

- Developing flexible electronics that can be used in many innovative ways.
- Creating new methods for building novel DNA circuits that can be used for medical diagnostics.

The verdict is not yet in on the newer classes who are still conducting their research as fellows, but the expectation is that they will also produce major advances in science and technology.

The NSSEFF awardees from the first three classes were high-quality researchers, as indicated by the number of prestigious awards and honors that they have earned and the relative number of highly cited research publications they have produced. Many of the fellows have been recognized for their excellence by their peers through membership in the National Academy of Sciences or were elected as fellows in their respective professional societies. Most of the fellows have received merit-based awards from their respective societies or associations since they have become fellows. Across the board, the fellows have produced highly cited publications as demonstrated by their having a mean h-factor of 53.4, ranging from 17 to 134. Likewise, the fellows are regularly requested to perform in an advisory role for many government agencies (e.g., National Science Foundation, National Institute of Health, DARPA, and Department of Energy) in addition to continued work with the DoD labs.

The interviews with the awardees from the first three award classes yielded overwhelmingly positive comments. The fellows stressed how the length and value of the award allowed them to take calculated risks that frequently led to strong advancements in their field of research, with many "firsts" or increases in capabilities by multiple orders of magnitude. Several of the fellows stated that the funding led to patents and enabled the development of new manufacturing processes that led to new spin-off companies that are advancing state-of-the-art technology development.

One of the conclusions we drew from our interviews of the initial three classes was the initial lack of an organized interaction with DoD scientists and/or laboratories. Even though many had an established relationship with the DoD or became involved as a result of this fellowship there were some fellows who were disappointed in the fact that they did not have a formal opportunity to interact with DoD scientists and they felt that this was one weakness in the program. This has been rectified for the most recent fellows as a new program, the Laboratory University Collaboration Initiative, was recently created in 2016. LUCI funds DoD Laboratory scientists to work in collaboration with the Vannevar Bush Fellows. This program provides a critical link between the fellows and DoD laboratories. In the future it would be extremely beneficial to the fellows if a similar link can be established with Industry, particularly the major DoD contractors. This would further ensure that the results of the research would be readily available to those entities that can best utilize them.

Many of the awardees also indicated that the award allowed the fellow to support quality graduate students who have subsequently joined the DoD research force since graduating (i.e., working for a DoD lab or acting as a PI on a DoD funded project). Because the fellowship funding was consistent over several years this enabled the awardees to offer year-after-year funding to talented graduate students and post-doctoral researchers, a big incentive. The skills gained by these students and researchers in the fields of research that are important to DoD helps seed the future workforce that DoD can draw upon.

This program has evolved significantly over the last decade. The first two classes were exposed to a novel selection process that included an in-person panel interview process that the awardees really appreciated. Several scientists considered the panel interview a significant life event. The remainder of the classes were selected by a more traditional process i.e., white paper, down-selection, proposal, review and final selection. Other changes to the program include the expectation of security clearances, with the original classes being expected to obtain a clearance while with current classes the application for a clearance is not required.

There was a significant break in new awards during the 2011–2013 timeframe because of the transition of the VBFF (NSSEFF) program to the OSD STEM Education Office that did not have the technical leadership at that time to manage it. However, in 2014 the program was returned to the Basic Research Office and was revitalized into a very significant part of the OSD Basic Research portfolio and has made new awards each year with the goal of having at least 50 concurrent awards at any given time. In 2016, the LUCI awards were instituted to provide a strong link to the DoD Laboratories.

The review of DoD Basic Research by the National Research Council (2005) warned that limiting unfettered exploration through research (historically a critical enabler of important breakthroughs) could limit the effectiveness of research efforts. The VBFF is a program that is designed to provide the freedom for awardees to explore, and that has led to important advancements and is expected to continue to enable scientific breakthroughs in domains that are important to DoD.

In *The Endless Frontier* (1945), Vannevar Bush laid out five fundamental principles to foster support for scientific research: (1) stability of funds over years to sustain long-range programs, (2) agency oversight by individuals with understanding of scientific research, (3) use of grants or contracts to fund research, (4) independence of universities and research institutes for specifics of conducting research, and (5) only high-level oversight of research efforts. The VBFF meets all of these principles, in that it provides considerable funds over a relatively long period of years that enable the researchers at universities to explore particular domains of science that are important to DoD. The assessment of proposals, administration, and oversight of the research efforts is conducted by individuals who understand the research, but the oversight burden to awardees is kept to a minimum. The renaming of this program in honor of Vannevar Bush is appropriate because it is conducted in accordance with his vision for fostering quality research that is important for the nation's long-term security needs.

C. Recommendations

- To keep the award prestigious and highly competitive, maintain funding for approximately 50 concurrent fellows (i.e., 10 new awards each year).
- To promote exploration and flexible research to make significant breakthroughs, continue to allow the fellows to adjust research plans as they progress.
- To maintain attractiveness of fellowship, maintain high level of funding and only high-level oversight (low burden).
- To leverage research capabilities developed through the fellowship, develop alumni group that maintains ongoing links to DoD laboratory research and scientists.
- To leverage skills gained by graduate students and post-doctoral researchers, explore methods for increasing their participation in future DoD research efforts (e.g., working for DoD, applying for future DoD research grants, working for DoD contractors).
- To expand dissemination of research advancements, increase efforts to promote research findings to industries crucial to DoD.
- To maintain technical expertise in the selection of fellows, leverage academic and industry expertise for proposal review process and consider a return to a distinguished panel of experts for final review.

Appendix A.
Summaries of Fellows (2008–2010)

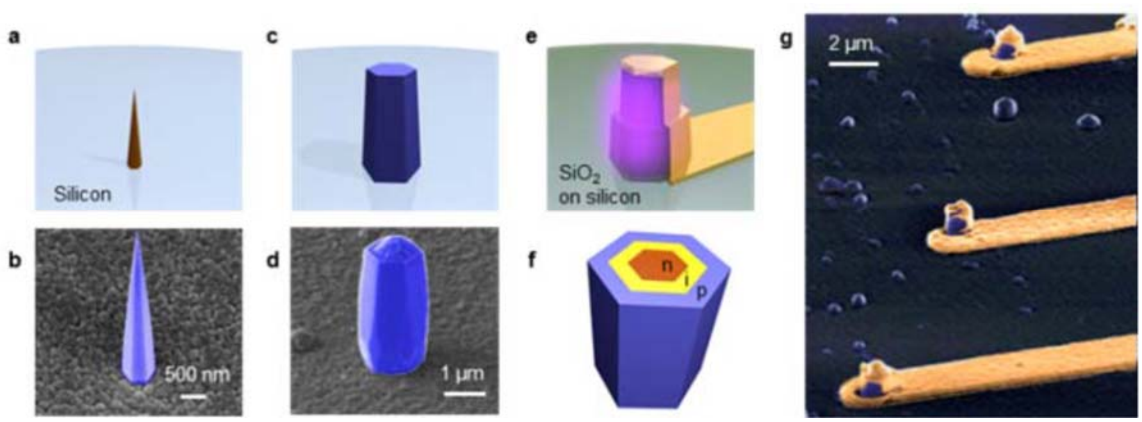
NSSEFF Awardee: Constance Chang-Hasnain **Year of Award:** 2008

Project Name: Nanostructured Materials for Low Power, Low Weight, High Performance Electronic and Optoelectronic Devices

Dr. Constance Chang-Hasnain, the John R. Whinnery Distinguished Chair Professor from the Electrical Engineering and Computer Science Department at the University of California, Berkeley, was awarded an NSSEFF grant in 2008 to provide a comprehensive program on advanced nanomaterials research and to demonstrate a set of devices that would advance sensing, processing, and communication capabilities. The vision of this project was to investigate novel nanomaterials synthesis and nano-optoelectronic devices to achieve energy-efficient lightweight and compact integrated microsystems by tailoring material properties using nanostructures to provide capabilities that could not be achieved otherwise.

Achievements: One of the key achievements of this research was to develop new growth methods for growing III-V semiconductors (e.g., (In, Al)GaAs and In(Ga)P) on silicon substrates. This monolithic integration is crucial for enabling high-performance optical components like light-emitting diodes (LEDs), lasers, and amplifiers to be grown directly on silicon complementary metal oxide semiconductor (CMOS) electronic circuits.

Figure 1 illustrates this novel technique for growing III-V semiconductors on silicon.



Source: Gimm (2013)

Figure 1. Bottom-up Integration of III-V Nano-optoelectronics on Silicon. Through core-shell growth, nano-needles can transform into nanopillars that form the basis of our nano-optoelectronic devices. (a) A schematic and (b) a scanning electron microscope (SEM) image of a GaAs-based nano-needle grown directly on silicon. (c) A schematic and (d) SEM image of a nano-pillar. (e) A schematic of a nano-pillar-based device integrated on silicon, made possible by radial p-i-n heterojunctions that form within nano-pillars as schematized in (f). (g) An SEM image shows a fabricated array of nano-pillar-based devices, demonstrating bottom-up opto-electronic integration on silicon

This technique shown in Figure 1 has led to the demonstration of the first optically pumped nano-laser, a single-pillar solar cell, and the first LED directly grown on silicon. This work was chosen for cover stories of *Nature Photonics* and *Applied Physics Letters* and won Best Student Paper Awards at two major international conferences.

There were also some unexpected discoveries that came from the unfettered research provided by NSSEFF. A new class of flat, ultra-thin optics using high-refractive-index contrast gratings had some extraordinary properties that allowed her to develop the fastest tunable vertical cavity surface emitting lasers (VCSELs). These gratings can also be used for ultra-thin planar lenses and focusing reflectors that can be used to split or route light. Because these gratings were so thin, they were flexible, which led to another unexpected use of these gratings—an artificial "chameleon" skin that would change color by stretching or electrical stimulation. Dr. Chang-Hasnain is continuing this work and is supported by the DoD, Department of Energy, and National Science Foundation (NSF).

Representative Publications

Chang-Hasnain, C. J., and W. Yang. 2012. "High-Contrast Gratings for Integrated Optoelectronics." *Advances in Optics and Photonics* 4, no. 3: 379–440.

Chen, R., T.-T. D. Tran, K. W. Ng, W. S. Ko, L. C. Chuang, F. G. Sedgwick, and C. Chang-Hasnain. "Nanolasers Grow on Silicon." 2011. *Nature Photonics* 5, no. 3: 170–175.

Chuang, L. C., F. G. Sedgwick, R. Chen, W. S. Ko, M. Moewe, K. W. Ng, T.-T. D. Tran, and C. Chang-Hasnain. 2011. "GaAs-Based Nanoneedle Light Emitting Diode and Avalanche Photodiode Monolithically Integrated on a Silicon Substrate." *Nano Letters* 11, no. 2: 385–390.

Chuang, L. C., M. Moewe, K. W. Ng, T.-T. D. Tran, S. Crankshaw, R. Chen, R., W. S. Ko, and C. Chang-Hasnain. 2011. "GaAs Nanoneedles Grown on Sapphire." *Applied Physics Letters* 98, no. 12: 123101

Ren, F., K. W. Ng, K. Li, H. Sun, and C. J. Chang-Hasnain. "High-Quality InP Nanoneedles Grown on Silicon." 2013. *Applied Physics Letters* 102, no. 1: 012115

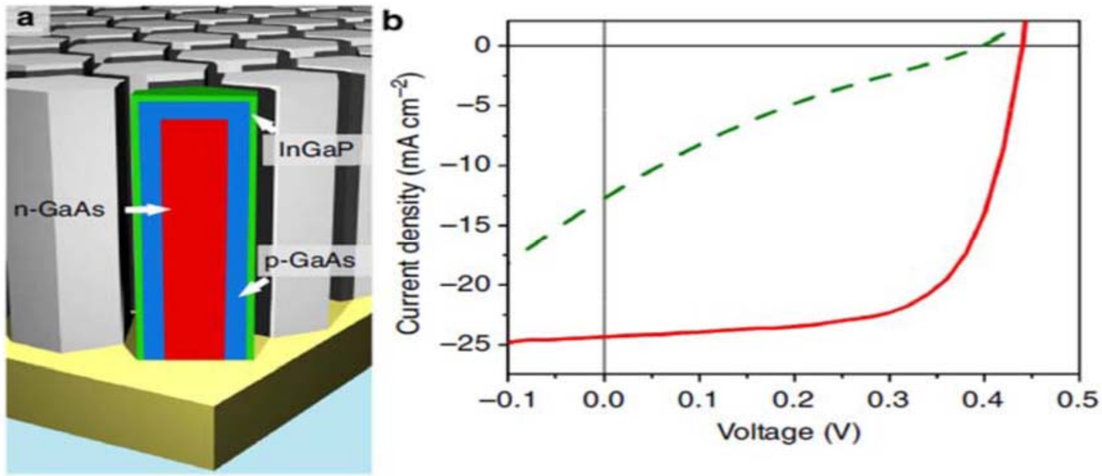
NSSEFF Awardee: Diana L. Huffaker **Year of Award:** 2008

Project Name: Exploring Dissimilar and Nano-Materials Integration as a Platform for New MWIR Device Functionality

Dr. Diana L. Huffaker, a professor in Electrical Engineering Department of the University of California Los Angeles, was awarded an NSSEFF Fellowship in 2008 to explore a novel approach for the integration of dissimilar and nanoscale materials that can lead to new functionality for optoelectronic devices. The key was to utilize group III-V (e.g., GaAs) semiconductor nano-pillars (NPs) integrated with dissimilar materials that cannot be combined using a conventional planar approach. This approach has led to the demonstration of low-threshold, continuous-wave photonic crystal lasers, low-noise, high-speed, plasmonically enhanced avalanche photodetectors, and low-cost, high-efficiency solar cells.

Achievements: One of the most significant accomplishments of this project was the ability to successfully realize high-quality NPs and NP heterostructures with different III-V semiconductors that can cover a wide range of the IR spectrum. Vertical NPs are grown on patterned substrates by *catalyst-free, selective-area epitaxy* using a metal-organic chemical vapor deposition reactor. Much effort has been devoted to understand and better control NP axial and lateral heterostructure formations. Through first-principle calculations using density function theory (DFT) and carefully designed experiments, Huffaker's team was able to achieve lattice-matched and dissimilar NPs and NP heterostructures, including a wide variety of materials combinations with the group-III (Ga, In) and group-V (As, P, Sb) elements. Furthermore, the team has demonstrated precise control over the position, geometry, and dimension of the NPs to form highly uniform NP arrays. Manipulating these degrees of freedom has allowed them to probe new functionalities in optoelectronic devices, such as light trapping, self-aligned plasmonic gratings, and creating photonic crystals, using a purely bottom-up approach.

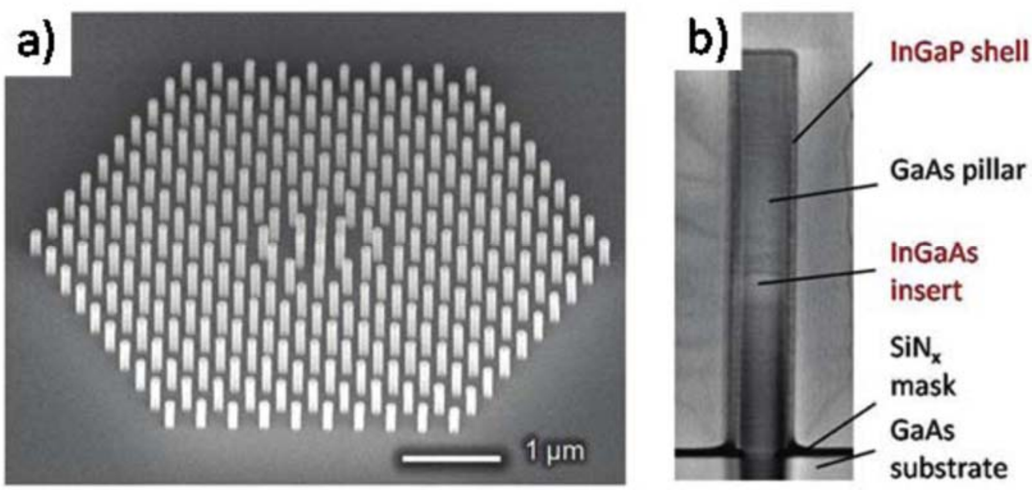
Using these techniques, the Huffaker team has demonstrated a three-dimensional GaAs solar cell array using a core shell p-n junction to increase the junction area for light collection. The use of the core shell approach to passivate the surface of the GaAs using an in-situ InGaAs shell was a major contributor to the improved performance of these cells and is attributable to the work on the optimization of the growth of the dissimilar materials described above. Figure 2 illustrates a schematic of the solar cell array and its I-V characteristic.



Source: Gimm (2013)

Figure 2: (a) Schematic Drawing of the GaAs Radial p-n Junction with InGaP Passivation Shell (not to scale). (b) Current density voltage characteristics under air mass 1.5 global illumination conditions with (solid red line) and without (dashed green line) InGaP passivation.

The Huffaker team has also demonstrated a photonic crystal laser using a precisely patterned array of NPs to form the photonic band-gap cavity as each NP is an axial heterostructure that forms the active gain medium. This is shown in Figure 3.



Source: Gimm (2013)

Figure 3: (a) A tilted SEM of an NP photonic crystal array as grown on the substrate. (b) Cross-section STEM of an NP showing the InGaAs insert located at the center of the pillar and InGaP shell.

The final significant accomplishment was the demonstration of a plasmonically enhanced NP *avalanche photodetector*. The NPs were used as a mask to form a nano-hole lattice that acts to plasmonically enhance the photon absorption in the NP array.

Representative Publications

Lin, A., J. N. Shapiro, A. C. Scofield, B. L. Liang, and D. L. Huffaker. 2013. "Enhanced InAs Nanopillar Electrical Transport by In-Situ Passivation." *Applied Physics Letters* 102, no. 5: 053115.

Mariani, G., A. C. Scofield, C.-H. Hung, and D. L. Huffaker. 2013. "GaAs NAnopillar-Array Solar Cells Employing In Situ Surface." *Nature Communications* 4: Article 1497.

Scofield, A. C., S.-H. Kim, J. N. Shapiro, A. Lin, B. L. Liang, A. Scherer, and D. L. Huffaker. 2011. "Bottom-up Photonic Crystal Lasers." *Nano Letters* 11, no. 12: 5387–5390.

Senanayake, P., C.-H. Hung, J. Shapiro, A. Lin, B. Liang, B. S. Williams, and D. L. Huffaker. 2011. "Surface Plasmon-Enhanced Nanopillar Photodetectors." *Nano Letters* 11, no. 12: 5279–5283.

Shapiro, J. N., A. Lin, P. S. Wong, A. C. Scofield, C. Tu, C. P. N. Senanayake, G. Mariani, B. L. Liang, and D. L. Huffaker. 2010. "InGaAs Heterostructure Formation in Catalyst-Free GaAs Nanopillars by Selective-Area Metal-Organic Vapor Phase Epitaxy." *Applied Physics Letters* 97, no. 4: 243102.

NSSEFF Awardee: Stephen I. Mayo **Year of Award:** 2008

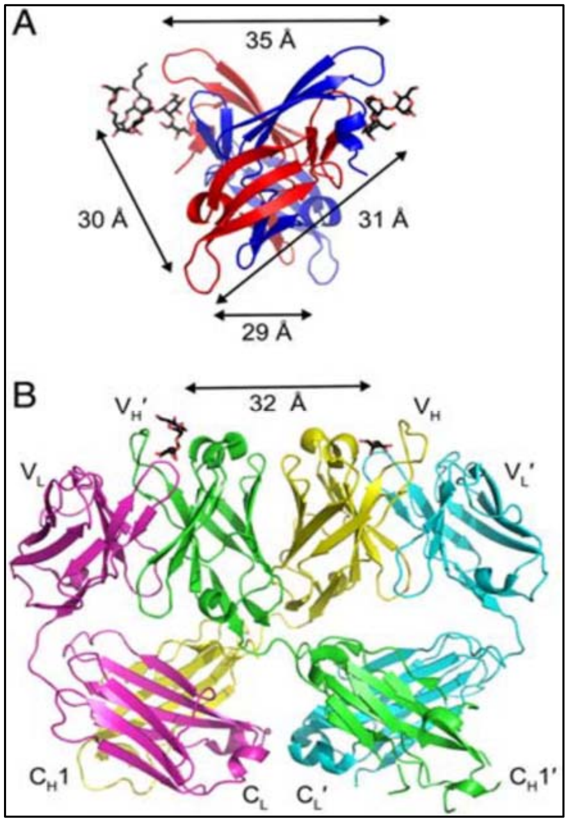
Project Name: Engineering Proteins for Anti-Viral Applications

Dr. Stephen I. Mayo, the Bren Professor of Biology and Chemistry and the William K. Bowes Jr. Leadership Chair, Division of Biology and Biological Engineering of the California Institute of Technology, Pasadena, CA, was awarded an NSSEFF Fellowship in 2008. This project revolved around the development and use of structure and computation-based protein design to engineer proteins with broad-spectrum antiviral activity. Traditional avenues for the prevention (e.g., vaccination) and treatment of viral infection (e.g., antiviral medications) are routinely overcome by the natural evolution of viral antigens.

Achievements: Mayo developed two classes of engineered proteins that by design are less susceptible to changes in viral antigens. First, computationally designed, multi-specific antibodies provide a route to antibody-based therapies that can accommodate the known and potential future evolution of targeted viral antigens. Second, enhanced lectins (i.e., proteins that bind carbohydrates) provide a route to target the carbohydrate chains on the glycoproteins of enveloped viruses that are difficult to manipulate by viral sequence evolution. In addition, to achieve a completely novel mode of therapeutic action for viral neutralization, Mayo proposed and developed a new class of therapeutic protein, called a "lectibody," that combines the carbohydrate binding ability of a lectin with the immune system activating ability of a particular region of an antibody.

As a result of the NSSEFF award, Mayo's team designed a bound form of the dimer Cyanovirin-N (CV-N), where CV-N is a small, naturally occurring lectin that has been shown to neutralize many enveloped viruses, including HIV. This form of the dimer was designed through an engineered tandem repeat (CVN2). CVN2 shows improved HIV neutralization activity by up to eighteen-fold compared with wild-type CV-N and shows broad cross-strain HIV neutralization, both likely due to CVN2's enhanced binding to gp120, an HIV envelope glycoprotein (Keeffe et al. 2011). The X-ray crystal structure of CVN2 revealed a domain-swapped dimer structure similar to wild-type CV-N that positions carbohydrate binding sites at distances similar to those on 2G12, a previously described anti-HIV antibody. This is illustrated in Figure 4, with the development of broad cross-strain HIV neutralization exhibited by these CV-N variants holds promise for future therapies.

Mayo's work on protein structure may lead to innovative methods for producing beneficial proteins that can be used for a broad range of purposes. In addition to his work on cyanovirin-based antiviral proteins, he leveraged NSSEFF funding to make advances in several areas of protein design: demonstrating the utility of using large structural ensembles for computational protein design (Allen et al. 2010); developing a new computational method called GRID for high-resolution protein structure refinement (Chitsaz and Mayo 2013); solving the structure of *Hypocrea jecorina* Cel5A, cellulose, an enzyme that is important for the conversion of cellulosic material to biofuels (Lee et al. 2011) and using computational protein design to generate Cel5A variants with enhanced thermal properties; and utilizing computational protein design to enhance the neutralization potency of antibodies against influenza.



Source: Gimm (2013)

Figure 4. Similarity of Carbohydrate Binding Site Spacing in Domain-swapped Dimer of CVN-N (A) and 2G12 (B).

Representative Publications

Allen, B. D., A. Nisthal, and S. L. Mayo. 2010. "Experimental Library Screening Demonstrates the Successful Application of Computational Protein Design to Large Structural Ensembles." *Proceedings of the National Academy of Sciences* 107 (46): 19838–19843.

Chitsaz, M., and S. L. Mayo. 2013. "GRID: A High-Resolution Protein Structure Refinement Algorithm." *Journal of Computational Chemistry* 34 (6): 445–450.

Keeffe, J. R., P. N. Gnanapragasam, S. K. Gillespie, J. Yong, P. J. Bjorkman, and S. L. Mayo. 2011. "Designed Oligomers of Cyanovirin-N Show Enhanced HIV Neutralization." *Proceedings of the National Academy of Sciences* 108 (34): 14079–14084.

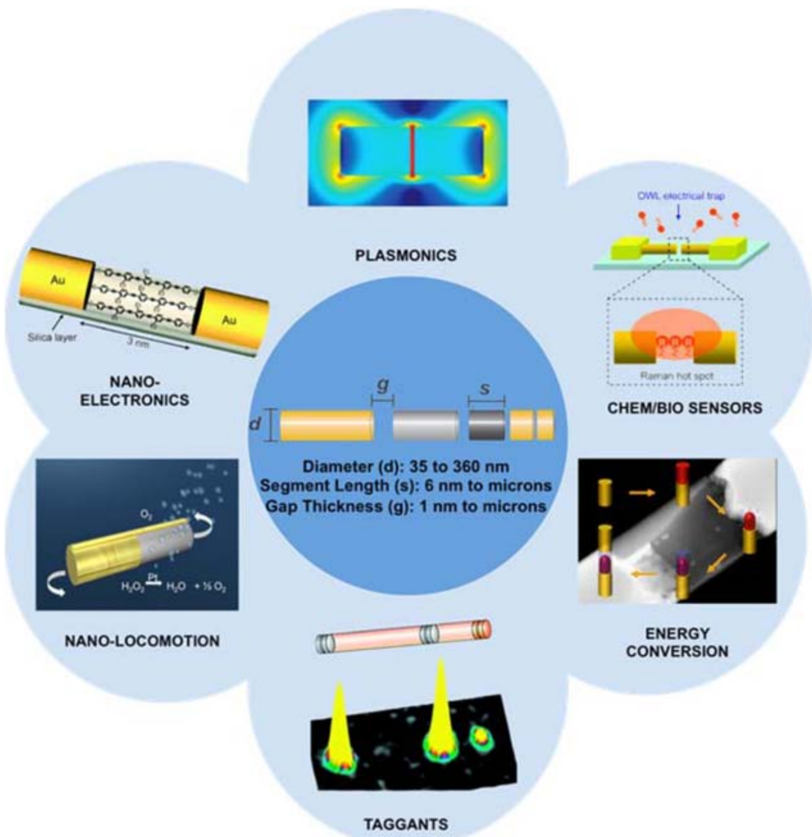
Lee, T. M., M. F. Farrow, F. H. Arnold, and S. L. Mayo. 2011. "A Structural Study of *Hypocrea Jecorina* Cel5A." *Protein Science* 20 (11): 1935–1940.

Privett, H. K., G. Kiss, T. M. Lee, T. M., R. Blomberg, R. A. Chica, L. M. Thomas, D. Hilvert, K. N. Houk, and S. L. Mayo. 2012. "Iterative Approach to Computational Enzyme Design." *Proceedings of the National Academy of Sciences* 109 (10): 3790–3795.

NSSEFF Awardee: Chad Mirkin **Year of Award**: 2008

Project Name: Functional One Dimensional Structures Based Upon On-Wire-Lithography

Dr. Chad Mirkin, the George B. Rathmann Professor of Chemistry at Northwestern University and the Director of the International Institute for Nanotechnology, was awarded an NSSEFF grant in 2008 for a project focused on a unique method for preparing one-dimensional heterostructures by a novel electrochemical technique called on-wire-lithography (OWL). This method was discovered by Prof. Mirkin and his group a few years before the onset of this project, and the goal of this effort was to fully define and explore the design space possible using OWL. Further, they desired to use the capabilities of OWL to synthesize and fabricate functional architectures that can have an impact on many fields including plasmonics, chemical and biological sensors, energy conversion, taggants, nano-locomotion and nano-electronics (see Figure 5).



Source: Gimm (2013)

Figure 5. Application Areas for OWL

Achievements: The Mirkin team established some of the limits of this technology, and they are impressive. The team was able to produce OWL nanostructures with diameters as small as 35 nm (about 1/1000 the diameter of a human hair), disk sizes along the wire with thicknesses of 6 nm, and gap sizes down to less than 1 nm. Furthermore, the team developed a set of tools that can be used by other researchers to develop and position new nanomaterials. This toolset included a unique set of nano-tweezers. With these tools and metrics in mind, the Mirkin team was able to demonstrate several unique device demonstrations:

- Unique plasmonic structures of coupled gold dimers with gap spacings from 0 to16 nm. These structures enabled the team to explore plasmonic coupling over a very wide range of parameters.
- Spectroscopy of single or small collections of molecules. By replacing the gap with organic molecules, these molecules could be explored by surface enhanced Raman spectroscopy (SERS). This ability to spectroscopically identify single or small collections of molecules has solved one of the major challenges in nanoscience.
- Demonstration of a core shell organic/semiconductor heterojunction photodetector with built in metallic leads with performance comparable to the best reported thin films photodetectors consisting the same organic/semiconductor heterojunction.
- Using disks of Au or Ag or both along an OWL-based wire, taggants can be fabricated that can store very dense coded information that can be read out using radio frequency (RF) excitation.
- Using nanorods of Pt–Au with compositional asymmetry, and using the catalytic decomposition of H_2O_2 with the concomitant formation of O_2 on the surface of the Pt segment, the nanorod would rotate. This could be the basis of nanomechanical devices for microfluidics and drug delivery.
- Building molecular electronic devices using click chemistry inside the gap between metallic segments. A diode-like response was clearly demonstrated.

The Mirkin group published 51 articles directly related to OWL, 42 of them after the start of the NSSEFF funding. These papers have been cited over 1600 times, and the number of papers by others on these topics significantly increased starting in 2011, with a total of 66 papers and 800 additional citations. The citation rate for all of these papers is continuing to rise dramatically.

Professor Mirkin has worked and continues to work with the Air Force (presumably the Air Force Office of Scientific Research (AFOSR)), and one of his students Abrin Schmuker is now working at the Air Force Research Laboratory at Wright Patterson Air Force Base. This project has enabled the Mirkin group to establish and build ongoing relationships with the DoD and the DoD labs, particularly the Air Force Research Laboratory.

Representative Publications

Banholzer, M. J., K. D. Osberg, S. Li, B. F. Mangelson, G. C. Schatz, and C. A. Mirkin. "Silver-Based Nanodisk Codes." 2010. *ACS Nano* 4, no. 9: 5446–5452.

Chen, X. D., A. B. Braunschweig, M. J. Wiester, S. Yeganeh, S., M. A. Ratner, and C. A. Mirkin. “Spectroscopic Tracking of Molecular Transport Junctions Generated by Using Click Chemistry.” 2009. *Angewandte Chemie International Edition* 48, no. 28: 5178–5181.

Osberg, K. D., A. L. Schmucker, A. J. Senesi, and C. A. Mirkin. “One-Dimensional Nanorod Arrays: Independent Control of composition, Length, and Interparticle Spacing with Nanometer Precision.” 2011. *Nano Letters* 11, no. 2: 820–824.

Osberg, K. D., M. Rycenga, N. Harris, A. L. Schmucker, M. R. Langille, G. C. Schatz, and C. A. Mirkin. 2012. “Dispersible Gold Nanorod Dimers with Sub-5 nm Gaps as Local Amplifiers for surface-Enhanced Raman Scattering.” *Nano Letters* 12, no. 7: 3828–3832.

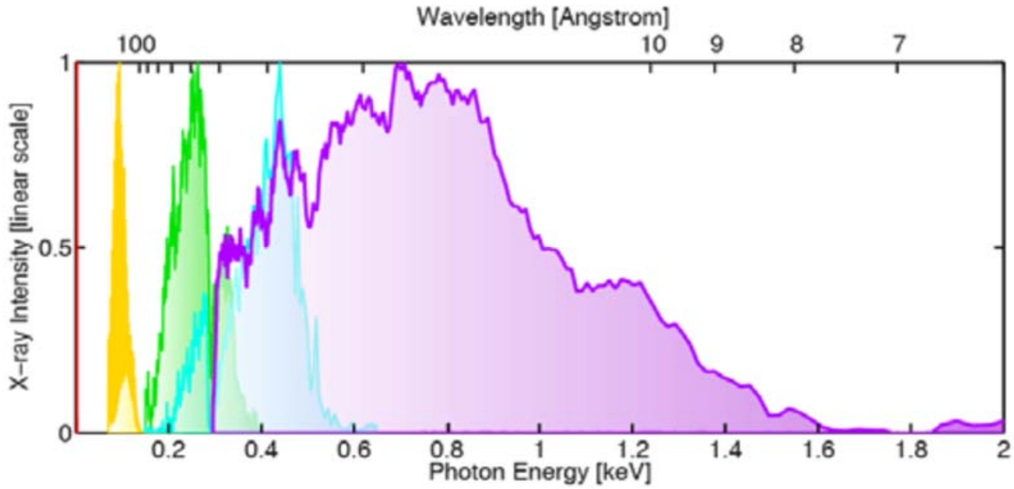
Wei, W., S. Li, S. Z., J. E. Millstone, M. J. Banholzer, X. Chen, X. Xu, G. C. Schatz, and C. A. Mirkin. 2009. “Surprisingly Long-Range Surface Enhanced Raman Scattering (SERS) on Au-Ni Multisegmented Nanowires.” *Angewandte Chemie International Edition* 48, no. 23: 4210–4212.

NSSEFF Awardee: Margaret M. Murnane **Year of Award:** 2008

Project Name: Development of High Power Ultrafast Lasers and Applications in Hyperspectral Imaging and Nanotechnology

Dr. Margaret M. Murnane, Professor of Physics at the University of Colorado, was awarded an NSSEFF fellowship in 2008 to: (1). Develop a new approach to generate ultrashort, high-intensity pulses in the mid-infrared (1.4 to 4 microns) region of the spectrum that will enable the ionization of matter and the exploration of new, strong field quantum physics. (2) Explore coherent X-ray generation from atoms driven by ultrafast mid-infrared lasers that would enable new applications for nano-imaging, nanoscience, and nanotechnology. Before this NSSEFF award, the underlying quantum physics for these predictions of X-ray generation had not been verified. (3) Harness coherent diffraction imaging to implement a new tabletop imaging capability using soft X-rays that enables image reconstruction without using an imaging lens.

Achievements: The most dramatic accomplishment of the NSSEFF project was to show that the quantum physics of how atoms ionize in strong laser fields can be combined with extreme nonlinear optics to produce coherent, tabletop light sources in the X-ray region of the spectrum for the first time. This solved the long-standing challenge of how to convert laser light into the X-ray region, to regimes not even imagined before the NSSEFF work. This was done by using the extreme nonlinear-optical process of high harmonic generation (HHG), where light from an ultrafast laser can be coherently upshifted in frequency to produce the extreme UV to X-ray light. The process involves an electron ionized by a quantum tunneling process. This electron undergoes nonlinear motion acting as a nanoscale radiating dipole that radiates very short wavelength (X-ray) light. Since these X-rays can penetrate thick samples and image with elemental and chemical specificity, this can be a turned into a new tool to visualize a host of technologically important nanoscale systems (see Figure 6).



Source: Gimm (2013)

Figure 6. HHG from Tabletop Ultrafast Lasers is a Unique Light Source, Generating Coherent Beams that Span Multiple X-ray Absorption Edges in Atoms. Using this source, nanoscale dynamics can be captured with elemental and chemical specificity, since the positions of these edges are sensitive to the local environment. The different colored spectra correspond to different driving laser wavelengths.

Representative Publications

Andriukaitis, G., T. Balčiūnas, T., S. Ališauskas, A. Pugžlys, A. Baltuška, T. Popmintchev, M.-C. Chen, M. M. Murnane, and H. C. Kapteyn. 2011. "90 GW Peak Power Few-Cycle Mid-Infrared Pulses from an Optical Parametric Amplifier." *Optics Letters* 36, no. 16: 2755–2757.

Popmintchev, T, M. C. Chen, D. Popmintchev, P. Arpin, S. Brown, S. Ališauskas, G. Andriukaitis, T. Balčiūnas, O. D. Mücke, A. Pugzlys, et al. "Bright Coherent Ultrahigh Harmonics in the keV X-ray Regime from Mid-Infrared Femtosecond Lasers." 2012. *Science* 336, no. 6086: 1287–1291.

Popmintchev, T., M.-C. Chen, P. Arpin, M. M. Murnane, and H. C. Kapteyn. 2010. "The Attosecond Nonlinear Optics of Bright Coherent X-ray Generation." *Nature Photonics* 4, no. 12: 822–832.

Popmintchev, T., M.-C. Chen, A. Bahabad, M. Gerrity, P. Sidorenko, O. Cohen, I. P. Christov, M. M. Murnane, and H. C. Kapteyn. 2009. "Phase Matching of High Harmonic Generation in the Soft and Hard X-ray Regions of the Spectrum." *Proceedings of the National Academy of Sciences* 106, no. 26: 10516–10521.

Seaberg, M. D., D. E. Adams, E. L. Townsend, D. A. Raymondson, W. F. Schlotter, Y. W. Liu, C. S. Menoni, L. Rong, C. C. Chen, J. W. Miao, et al. 2011. "Ultrahigh 22 nm Resolution Coherent Diffractive Imaging Using a Desktop 13 nm High Harmonic Source." *Optics Express* 19, no. 23: 22470–22479.

NSSEFF Awardee: Carey E. Priebe **Year of Award:** 2008

Project Name: Fusion and Inference from Multiple and Massive Disparate Data Sources

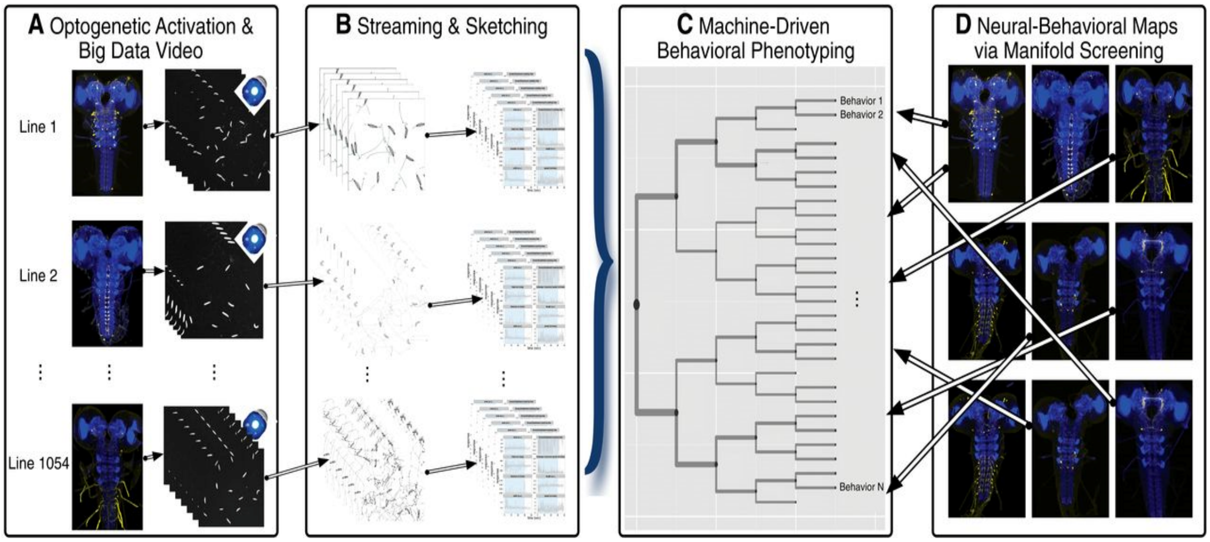
Dr. Carey Priebe, a professor in the Department of Applied Mathematics and Statistics at Johns Hopkins University, was awarded an NSSEFF grant in 2008 to address fusion and inference of "big data." Priebe defines big data not just as massive quantities of data, but as massive quantities of multiple data types from disparate sources. This could include text, video, speech, social network information, etc. that may be stored in different places. The goal of the research effort was to derive statistical pattern-recognition methods and tools to address difficulties with fusion and inference from multiple, massive, and disparate data sources.

Achievements: The Priebe team's research enabled by the NSSEFF award included developing a unifying algorithmic framework for fusing disparate data types across different domains (e.g., neuroscience, human trafficking, and image analysis), demonstrating how specific approaches within the framework provide quality fusion and inference from big data sets, and detecting change points that can signal important anomalies that might be hidden from standard analysis methods (Tang et al. 2013).

Some of this work was on the fusion of spatially structured information (e.g., brain/neuron signals) and physical behavior with relation to time. In an attempt to develop analysis tools to fuse disparate data Priebe and colleagues selected the task of mapping neuron functions as an example of "big data." For this effort, they optogenetically activated 1000+ brain neurons of the Drosophila (i.e., fruit fly) larvae systematically in 37,000 animals (Vogelstein et al. 2014). The larvae behavior that followed each activation instance was recorded, and the correlation between neuron activation and behavior was mapped through the use of multiscale unsupervised structure learning. This has led to the largest neuron/behavior mapping of an organism to date (C. Priebe, personal communication, 9 October 2015) and demonstrated that the analytical technique (see Figure 7) could be scaled to understand the brain/behavior connections of more complex organisms.

The analytic techniques Priebe developed can be used in different domains. For example, the NSSEFF-funded research laid the foundation for subsequent DoD research by Priebe for the XDATA program of the Defense Advanced Research Projects Agency (DARPA), where Priebe and colleagues used their methods to analyze graph data to account for unobserved information to make inferences. The robustness of the optimization schemes was illustrated with data examples, including social network activity, that led to identifying individuals involved in human-trafficking (Fishkind et al. 2015). Priebe's inference methods have also been used for quantitative horizon scanning to mitigate technological surprise (Priebe et al. 2012).

The research enabled through the Vannevar Bush Fellowship has been recognized beyond DoD. Priebe's fellowship funded research was one of the reasons he won the 2010 American Statistical Association Distinguished Achievement Award. The fellowship and the research it funded were also instrumental for obtaining a recent NSF Early Concept Grants for Exploratory Research (EAGER) award as part of the Federal Government's BRAIN Initiative.



Source: Gimm (2013)

Figure 7. Overview of Experimental Design and Methodology for Mapping Neuron–Behavior Connections, from Vogelstein et al. (2014). (A) Optogenetic activation or neurons and recording or neural actions; (B) extracting contour sketches to characterize animal motion; (C) machine-driven behavior labeling via multiscale unsupervised structure learning; and (D) manifold testing to determine which neurons evoke particular behaviors.

Representative Publications

Fishkind, D. E., V. Lyzinski, H. Pao, L. Chen, and C. E. Priebe. 2015. "Vertex Nomination Schemes for Membership Prediction." *The Annals of Applied Statistics* 9 (3): 1510–1532.

Priebe, C. E., J. L. Solka, D. J. Marchette, and A. C. Bryant. 2012. "Quantitative Horizon Scanning for Mitigating Technological Surprise: Detecting the Potential for Collaboration at the Interface." *Statistical Analysis and Data Mining* 5 (3): 178–186.

Tang, M., Y. Park, N. H. Lee, and C. E. Priebe. 2013. "Attribute Fusion in a Latent Process Model for Time Series of Graphs." *IEEE Transactions on Signal Processing* 61 (7): 1721–1732.

Vogelstein, J. T., Y. Park, T. Ohyama, R. A. Kerr, J. W. Truman, C. E. Priebe, and M. Zlatic. 2014. "Discovery of Brainwide Neural-Behavioral Maps via Multiscale Unsupervised Structure Learning." *Science* 344 (6182): 386–392.

NSSEFF Awardee: Barbara Shinn-Cunningham **Year of Award:** 2008

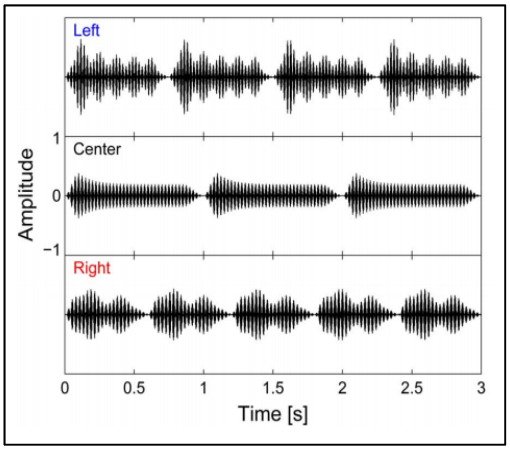
Project Name: Managing Acoustic Communications in High-Stress Environments

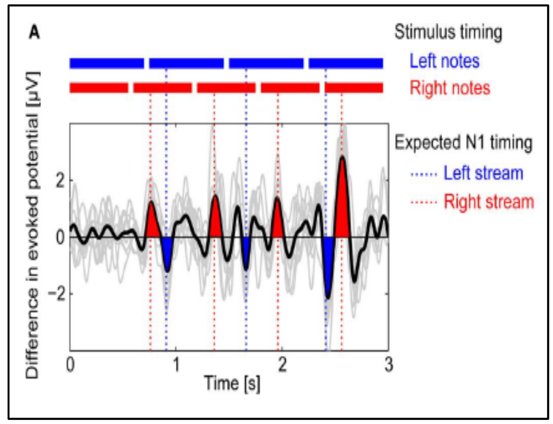
Dr. Barbara Shinn-Cunningham, Professor of Biomedical Engineering and the Director of the Auditory Neuroscience Lab at Boston University, was awarded an NSSEFF grant in 2008 to address auditory attention processes in the brain. In her research, she developed a method to identify which sound source a person was attending to through the use of electro-encephalography (EEG), a set of measurements of the voltages on the scalp generated from brain activity.

Achievements: The initial thrust was to develop methods to determine an observer's attention from noninvasive brain-imaging techniques and to use that information to improve the design of auditory feedback for display systems. By combining behavioral studies with noninvasive neuro-imaging studies the researchers could identify what auditory messages were being attended to or ignored (Bharadwaj, Lee, and Shinn-Cunningham 2014). The potential application of this research was clear for noisy command centers and other military environments where there are many potentially distracting sounds.

The research team developed a novel technique of having varying rhythms to the auditory signals, which allowed the researchers to look for EEG signals that temporally matched those rhythms. For example, over a 3-second span, one rhythm was four quivering tones, another was three consistent tones, and the last was five wavering tones (Figure 8a). In some experiments, subjects were asked to focus on the right or left tones, and through the EEG output it was possible to identify which of the tones the participant attended to (Figure 8b). These results revealed that focused auditory attention both enhances the response to an attended stream and suppresses the response to an unattended stream.

An unexpected outcome that came from this research was the development of a capability to test a person's hearing in such a way as to identify if the hearing difficulty was due to a sensory hearing loss or perceptual difficulty (Bharadwaj et. al. 2015). In some cases, the inability of some soldiers to comprehend speech in normal conditions months after being subjected to significant blast trauma was assumed to be linked to a sensory hearing impairment. Through previous testing methods like pure tone testing, it was not clear if a person who had difficulty comprehending speech had adequate sensory input to the brain (functioning of ears) or a cognitive impairment (functioning of the brain). The techniques developed by Shinn-Cunningham and colleagues allowed for a clear determination of where the functioning difficulty existed. The research has found that while a person may sense (i.e., generate a neural signal) for a tone that is consistent for a second or more as would be required during a pure tone test, they may not sense the subtle sound variations on the temporal scale of 1/100 second that are required to detect transitions from consonants to vowels that enable speech understanding. This research led to current work at Walter Reed to determine when difficulties in verbal comprehension that occur after a blast exposure are due to sensory hearing loss (i.e., inner ear and auditory nerve damage) versus diminishment of cognitive functioning.





(a) (b)

Source: Images from Choi et al. (2013).

Figure 8. (a) The auditory stimuli waveforms for each trial consisted of three sounds streams had a distinct rhythms (i.e., three, four, or five notes), a distinct timbre (i.e., cello, clarinet, or oboe), a pitch range that did not overlap with the other streams (high, middle, low), and a distinct lateral location (left, center, or right). (b) The onset of the signals induced a difference in evoked potential measured through EEG.

This research may lead to better diagnostic methods to more accurately address injuries by military personnel. One of Dr. Shinn-Cunningham's students, Adrian K. C. Lee, now an Associate Professor at the University of Washington, won an AFOSR Young Investigator Research Program Award for his work integrating neuroscience and engineering approaches to classifying human brain states. Dr. Lee has also collaborated with the Audiology and Speech Center at Walter Reed National Military Medical Center.

Representative Publications

Bharadwaj, H. M., A. K. Lee, and B. G. Shinn-Cunningham. 2014. "Measuring Auditory Selective Attention Using Frequency Tagging." *Frontiers in Integrative Neuroscience* 8 (Article 6): 1–12.

Bharadwaj, H. M., S. Masud, G. Mehraei, S. Verhulst, and B. G. Shinn-Cunningham, B. G. 2015. "Individual Differences Reveal Correlates of Hidden Hearing Deficits." *The Journal of Neuroscience* 35 (5): 2161–2172.

Choi, I., S. Rajaram, L. A. Varghese, and B. G. Shinn-Cunningham. 2013. "Quantifying Attentional Modulation of Auditory-Evoked Cortical Responses from single-Trial Electroencephalography." *Frontiers of Human Neuroscience* 7:115.

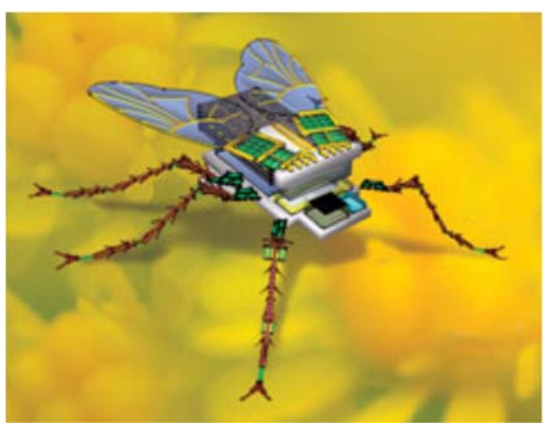
NSSEFF Awardee: Susan Trolier-McKinstry **Year of Award:** 2008

Project Name: High Strain Actuators for Miniaturized Actuators and Self-Powered Sensors

Susan Trolier-McKinstry, the Steward S. Flaschen Professor of Materials Science and Engineering and Electrical Engineering at the Pennsylvania State University, was awarded an NSSEFF fellowship in 2008 to develop (1) next-generation high-strain piezoelectric films; (2) robust processing methods that simplify patterning of complex oxides; and (3) integration strategies with a wide variety of substrates, including CMOS (complementary metal-oxide-semiconductors) and polymers.

Achievements: This research produced innovative processes that enabled the development of new materials with piezoelectric properties (Baek et al. 2011). Piezoelectric materials convert between electrical and mechanical energy in that mechanically straining the material produces an electrical signal, and introducing an electric field produces a mechanical deformation. This line of research has produced advanced materials and processing that enable breakthroughs in robotics, harvesting energy, and persistent surveillance.

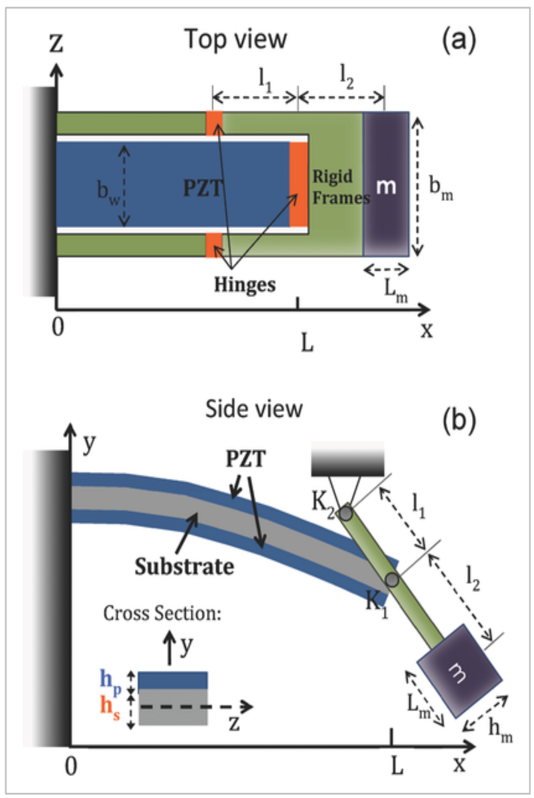
The development of new piezoelectric materials, as produced through this research, can be used for actuators in microelectromechanical systems (MEMS) to produce physical movement of very small parts, which will allow for smaller robotics systems. For example, the Army Research Laboratory recently produced piezoelectric actuating wings, similar to those of an insect, which can be used for very small flying surveillance platforms that would not be easily detected, as depicted in Figure 9. Such MEMS based on piezoelectric materials require minimal power to achieve motion, thereby allowing for lower overall weight of the MEMS. Through the NSSEFF grant, the development of epitaxial piezoelectric thin films produced a 50% gain in actuator strength compared with the then-current state-of-the-art materials.



Source: Eom and Trolier-McKinstry (2012)

Figure 9. An Example of How a Thin-film Piezoelectiric Could be Used to Power a Micro Drone in the Shape of a Fly.

One of the limitations to long-term deployment of sensors is a power source that would enable them to continue functioning for extended periods. Systems that can harvest energy from the environment can allow for persistent surveillance and sensing because they can generate their own power. When sound is prevalent in an area, the sound wave energy can be harvested through the use of piezoelectric films that convert the mechanical energy from the sound to an electrical output. Through the fellowship, Trolier-McKinstry was able to produce lead zirconate titanate (also known as PZT) films that output a nearly tenfold increase in power generated from the same quantity of aluminum nitride, which was the current standard material at the time. Sensors that are placed in noisy areas like bridges could be powered indefinitely through the sound vibrations, providing long-term assessment of the bridge or other infrastructure that requires long-term monitoring (Trolier-McKinstry et al. 2011).



Source: Yeo et al. (2016).

Figure 10. Schematic of an Energy-harvest Mechanism that Leads to up to 4× Greater Efficiency than a Standard Cantilevered Design because the New Design Subjects the PZT film to a More Uniform Bend Lengthwise.

In addition to the development of novel manufacturing processes for piezoelectric materials, the research effort led to collaborations with other research teams working in the field, which in turn has helped foster a critical mass of good researchers working in the area (Trolier-McKinstry et al. 2011). One such collaboration is a partnership with North Carolina State University to establish an NSF Engineering Research Center focused on nanoscale systems that integrate self-powered electronics for the advancement of personalized medicine. The program for Advanced Self-Powered Systems of Integrated Sensors and Technology (ASSIST) will create self-powered wearable systems that concurrently monitor a user's environment and health to potentially uncover links between exposure to pollutants and chronic diseases. Trolier-McKinstry's efforts for ASSIST will be developing energy harvesting and storage capabilities.

Representative Publications

Baek, S. H., J. Park, D. M. Kim, V. A. Aksyuk, R. R. Das, S. D. Bu, D. A. Felker, J. Lettieri, V. Vaithyanathan, S. S. N. Bharadwaja, et al. 2011. "Giant Piezoelectricity on Si for Hyperactive MEMS." *Science* 334 (6058): 958–961.

Eom, C. B., and S. Trolier-McKinstry. 2012. "Thin-Film Piezoelectric MEMS." *MRS Bulletin* 37 (11): 1007–1017.

Marincel, D. M., S. Jesse, A. Belianinov, M. B. Okatan, S. V. Kalinin, T. N. Jackson, and S. Trolier-McKinstry. 2015. "A-site Stoichiometry and Piezoelectric Response in Thin Film $PbZr_{1-x}Ti_xO_3$." *Journal of Applied Physics* 117 (20): 204104.

Trolier-McKinstry, S., F. Griggio, C. Yaeger, P. Jousse, D. Zhao, S. S. N. Bharadwaja, T. N. Jackson, S. Jesse, S. V. Kalinin, and K. Wasa. 2011. "Designing Piezoelectric Films for Micro Electromechanical Systems." *IEEE transactions on Ultrasonics, Ferroelectrics, and Frequency Control* 58 (9): 1782–1792.

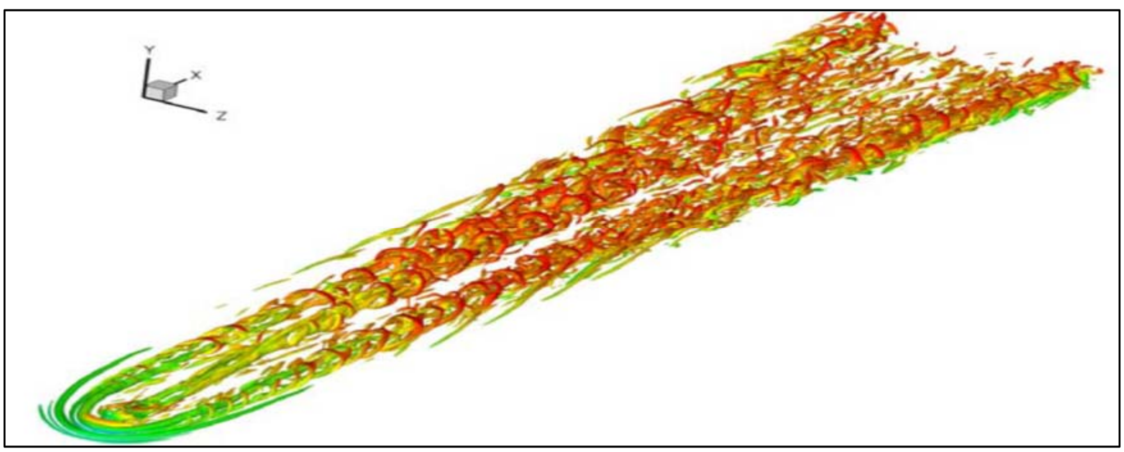
Yeo, H. G., X. Ma, C. Rahn, and S. Trolier-McKinstry. 2016. "Efficient Piezoelectric Energy Harvesters Utilizing (001) Textured Bimorph PZT Films on Flexible Metal Foils." *Advanced Functional Materials* 26 (32): 5940–5946.

NSSEFF Awardee: Graham V. Candler **Year of Award:** 2009

Project Name: Multi Physics Simulations of Hypersonic Flows

Dr. Graham V. Candler, the McKnight Presidential Professor in the Department Aerospace Engineering and Mechanics at the University of Minnesota, was awarded an NSSEFF grant in 2009 to develop new methods for addressing critical weaknesses in hypersonic flow simulations by developing new physical models, advanced numerical algorithms, and large-scale first-principles simulations. A key component of this proposed research was the emphasis placed on validating the simulation results using carefully designed experiments and Air Force flight experiments. One of the goals of this research was to significantly advance the computational fluid dynamics models of hypersonic flows to allow much more accurate designs of future hypersonic weapons systems.

Achievements: This research completely changed how fluid dynamics is done. The new numerical methods that were developed under this NSSEFF award allowed much more detail in the design. The older methods smoothed out interesting processes that were important to understand to complete an accurate design. Four topics in hypersonic flow physics were investigated: simulations of air-breathing scramjet engines operating at high Mach numbers (6–10), analysis of laminar-turbulent transitions, high-temperature processes, and shock-dominated flows.



Source: Gimm (2013)

Figure 11. Simulation of Boundary Layer Transition Due to a Discrete Roughness Element at Purdue Mach 6 Quiet Tunnel Conditions.

An example of this simulation work is illustrated in Figure 11. This figure demonstrates that a transition to turbulence may occur when there is a small, discrete roughness element protruding into the flow. The simulation that is illustrated here could not have been done with the older simulation tools in existence before this NSSEFF project. This figure is a visualization of the turbulent wake produced by a small cylindrical roughness element. Detailed comparison with the experiment carried out in the Purdue wind tunnel showed excellent agreement with the simulation, including predictions of the frequency of the primary instability and its harmonics.

The codes developed under this project are now used at more than 50 institutions, including all Air Force labs and the Naval Air Warfare Center. Furthermore, DARPA mandates the use of Candler's codes by Lockheed Martin, Northrup Grumman, and Boeing.

Representative Publications

Candler, G. V. 2010. "Comparison of CFD and Theoretical Post-Shock Gradients in Hypersonic Flow." *Progress in Aerospace Sciences* 46, nos. 2–3: 81–86.

Candler, G.V., P. K. Subbareddy, and I. Nompelis. 2013. "Decoupled Implicit Method for Aerothermodynamics and Reacting Flows." *AIAA Journal* 51, no. 5: 1245–1254.

Gronvall, J. E., H. B. Johnson, and G. V. Candler. 2012. "Hypersonic Three-Dimensional Boundary Layer Transition on a Cone at Angle of Attack." Paper presented at the 42nd AIAA Fluid Dynamic Conference, New Orleans, LA, 25–28 June 2012, AIAA 2012-2822.

Peterson, D. M., and G. V. Candler. 2011. "Simulations of Mixing for Normal and Low-Angled Injection into Supersonic Crossflow." *AIAA Journal* 49, no. 12: 2792–2804.

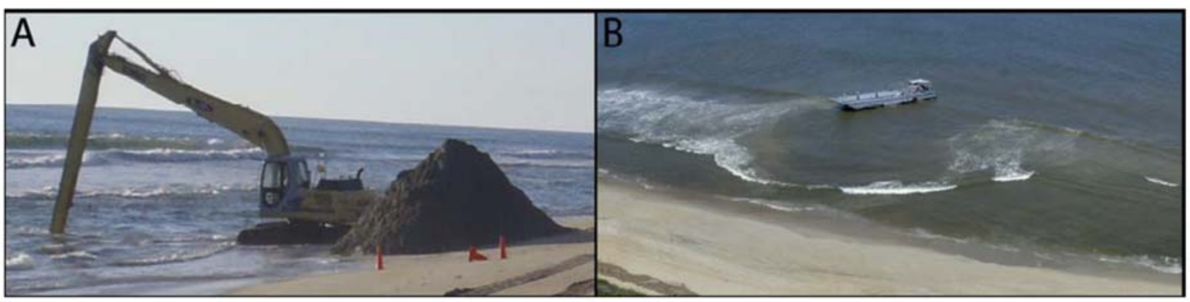
Wagnild, R., G. V. Candler, P. K. Subbareddy, and H. B. Johnson. 2012. "Vibrational Relaxation Effects on Acoustic Disturbances in a Hypersonic Boundary Layer over a Cone." Paper presented at the 50th AIAA Aerospace Sciences Meeting, including the New Horizons Forum and Aerospace Exposition, Aerospace Sciences Meetings, Nashville, TN, 09–12 June 2012, AIAA-2012-0922.

NSSEFF Awardee: Steve Elgar **Year of Award:** 2009

Project Name: Manipulating Nearshore Morphology to Determine the Coupling and Feedback between Waves, Currents, and Bathymetric Change

Dr. Steve Elgar, a senior scientist and physical oceanographer in the Applied Ocean Physics and Engineering Department at the Woods Hole Oceanographic Institution, was awarded an NSSEFF grant in 2009 to study the physics underlying the coupling and feedbacks between waves, currents, and sediment transport that cause morphological evolution of the seafloor mainly in the littoral zone or the region near the shore.

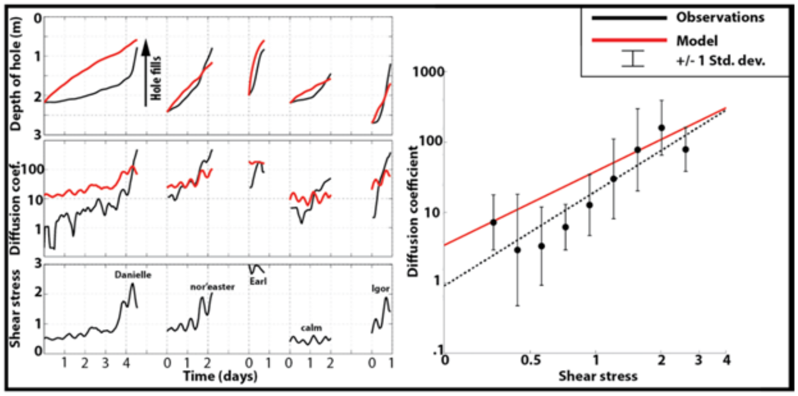
Achievements: To investigate this novel physics, Dr. Elgar and his students have been creating and monitoring perturbations to the seafloor in the surf zone where waves break. They have postulated that these perturbations produce storm-like gradients in hydrodynamics and morphology, thereby allowing them to investigate the evolution of these perturbations without having the need to maintain sensors during hurricanes. These perturbations are designed to address hypotheses with the goal of understanding the physics sufficiently to include the physics in the models generated in this project.



Source: Gimm (2013).

Figure 12. (A) A backhoe adjacent to a pile of sand excavated from the inner surf zone. The hole is beneath the long arm of the backhoe. (B) The propellers of the landing craft were used to dredge a channel across the inner surf zone. Waves refract differently over the deep water in the channel than over the shallower shoals on the sides of the channel, resulting in the curved wave crest onshore of the boat

To carry out this project Dr. Elgar and his PhD student Melissa Moulton excavated several big holes in the surf zone seafloor at the U.S. Army Field Research Facility, in Duck, NC (see Figure 12). Immediately after the excavation, they deployed wave and current sensors in and near the hole and surveyed the seafloor. The steep-sided holes, which are similar to steep features formed during storms, rapidly evolved during large waves from offshore hurricanes Danielle, Earl, and Igor, as shown in Figure 13. In contrast to the common assumption that gravity-driven transport is negligible, Melissa discovered that sediment transported by gravity (grains roll down hill) is the dominant mechanism refilling the steep holes, and thus is important during storms and should be included in models. The observations have allowed Melissa to develop a model for the gravity-driven transport (red curves in Figure 13) and to determine the diffusion coefficient as function of waves and currents.



Source: Gimm (2013)

Figure 13. (top left) Depth of the hole relative to ambient sand level (m) (arrow indicates the depth of the hole decreasing as the hole fills with sand), (middle left) diffusion coefficient (arbitrary units), and (bottom left) wave-current shear velocity (arbitrary units, an indication of the strength of wave-orbital velocities and mean currents) versus time for each of five holes. Black curves are observations and red curves are model predictions. Conditions that generated waves (and bottom shear stress) are labeled with storm names in (bottom left). (right) Diffusion coefficient versus shear velocity (arbitrary units) for observations (black) and model predictions (red). Vertical bars are ±1 standard deviation.

Representative Publications

Clark, D. B., S. Elgar, and B. Raubenheimer. 2012. "Vorticity Generation by Short-Crested Wave Breaking." *Geophysical Reearch Letters* 39, no. 24: L24604.

Elgar, S., B. Raubenheimer, J. Thomson, J. and M. Moulton. 2012. "Resonances in an Evolving Hole in the Swash Zone." *Journal Waterway, Port, Coastal, and Ocean Engineering* 138: 299–302.

Englestad, A., T. Janssen, T. H. C. Herbers, G. van Vledder, S. Elgar, B. Raubenheimer, L. Trainor, and A. Garcia-Garcia. 2012. "Wave Evolution across the Louisiana Shelf." *Continental Shelf Research* 52: 190–202.

Gast, R. J., L. Gorrell, B. Raubenheimer, and S. Elgar. 2011. "Impact of Erosion and Accretion on the Distribution of Enterococci in Beach Sands." Supplement. *Continental Shelf Research* 31: 1457–1461.

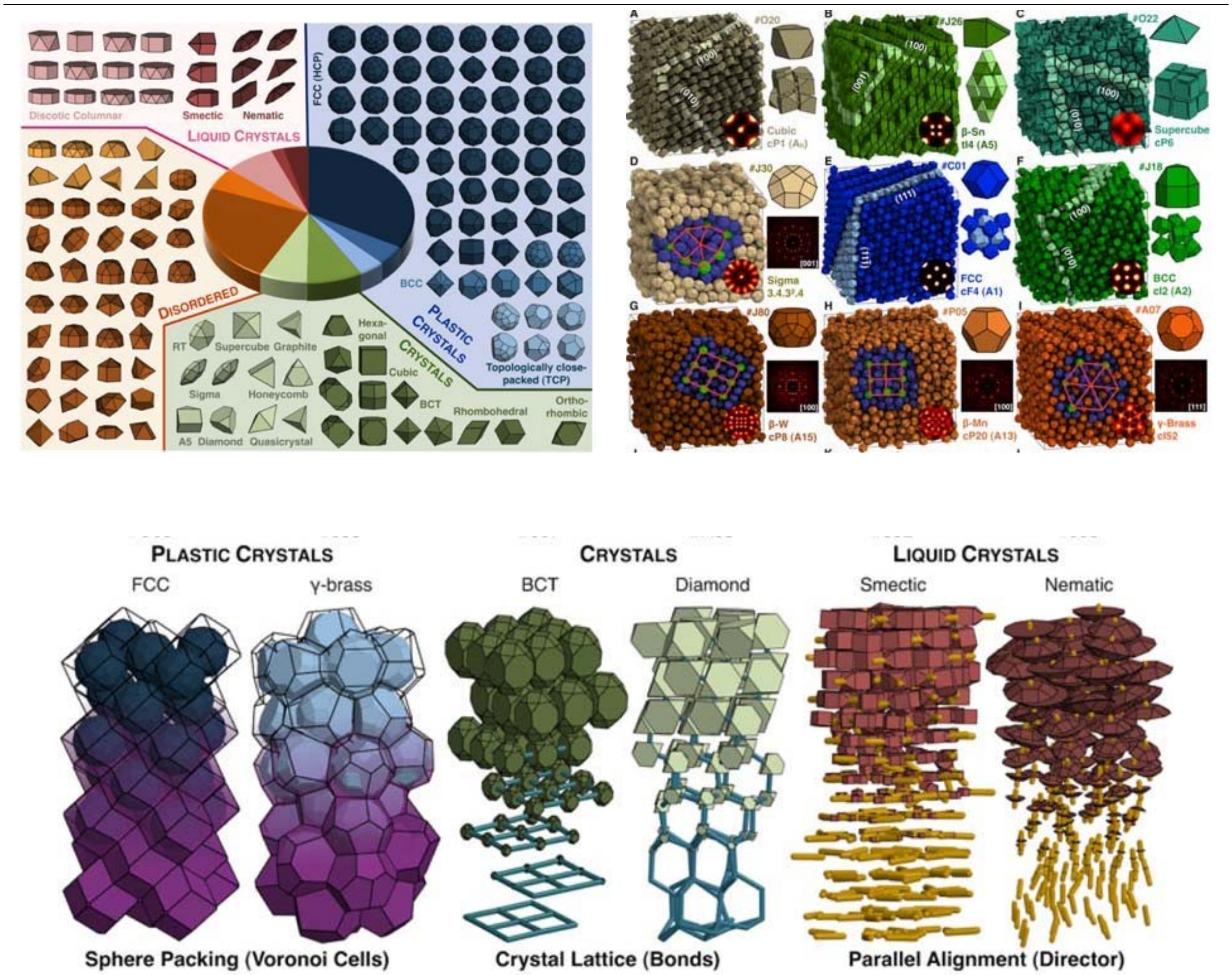
Raubenheimer, B.; D. Ralston, S. Elgar, D. Giffen, and R. Signell. 2012. "Observations and Predictions of Summertime Winds on the Skagit Tidal Flats, Washington." *Continental Shelf Research* 60: S13–S21.

NSSEFF Awardee: Sharon C. Glotzer **Year of Award:** 2009

Project Name: Smart, Autonomous, Adaptive Phenomena in Self organizing, Reconfigurable Materials

Dr. Sharon C. Glotzer, the John Werner Cahn Distinguished University Professor of Engineering and the Stuart W. Churchill Collegiate Professor of Chemical Engineering of the University of Michigan, was awarded an NSSEFF Fellowship in 2009. This award focused on developing an understanding of materials that can adapt to perform a host of important and novel functions either on demand or by responding to environmental cues. The goal was to produce materials that can perform molecular recognition, autonomously sense and report, or reconfigure to change shape or properties. This adaptability requires that the material's building blocks be able to assemble into target structures that can be "toggled" to other structures. The key objectives of this project include fundamental understanding of the relationship between building block complexity, assembly reconfigurability at nanometer to micron scales, designing and demonstrating *in silico* the self-assembly of target structures, and providing the first predictive simulation platform for designing and engineering pathways for assembly of nanoscale building blocks into complex target structures, including those capable of exhibiting the reconfigurability of adaptive materials.

Achievements: This NSSEFF award led to the discovery of some new insights about entropy and its role in how materials self-assemble. Glotzer's team discovered that entropy can produce "bonds" between nanoparticles as strong as typical chemical bonds. These bonds can be "directional" in the same way that hydrogen bonds and covalent bonds are between atoms and molecules. This discovery implies that entropy is far more important than previously thought in the formation of crystals made of nanoparticles. These "entropic bonds" are so important that entropy alone can be used to make highly ordered crystals with great structural complexity at the 1 nanometer to 1000 nanometer length scale, allowing for the prediction of new materials with unprecedented properties. Using a rapid computer-simulation-based screening approach, dozens of new crystal structures previously unseen for nanoparticles, but isostructural with known crystals made up of atoms and molecules, were found. Some of these structures and their building blocks are shown in Figure 14. Recently, to exploit the directionality of the entropic bonding, a new concept was proposed. Called *entropically patchy particles,* the concept directly relates shape, entropy and assembly in colloidal matter, revealing a deep connection between the shapes of nanoparticles and the structures they arrange into, giving materials researchers a new "knob" to turn in materials design and synthesis. This was a new design space for the self-assembly and dynamic reconfigurability of nanostructures based on entropic considerations. Prof. Glotzer has collaborated with many other groups, including other NSSEFF fellows that are utilizing the concepts developed in this project, including Prof. Chad Mirkin, who now has a second NSSEFF award. The predictions made by Dr. Glotzer's group are now guiding and influencing experimental research in the United States, Europe, and Asia.



Source: Damasceno, Engel, and Glotzer (2012).

Figure 14. A pictorial summary of the work under the NSSEFF program. Rapid, high-throughput computer simulations predicted assemblies for 145 different nanoparticle shapes (here, polyhedral shaped.) The four overarching categories of structures predicted include (indicated by different colors) liquid crystals, plastic (rotator) crystals, periodic and aperiodic crystals, and disordered (glassy) phases. Subcategories (classes) are indicated by shades. The assembly category of liquid crystals contains the classes discotic columnar, smectic, and nematic (different shades of pink). Plastic crystal classes are face-centered cubic (dark blue), body-centered cubic (blue), and topologically close packed (light blue). In the case of crystals, we distinguish Bravais lattices (dark green) and non-Bravais lattices (light green). RT stands for random tiling. For the glasses, no assembly is observed, and we distinguish those that strongly order locally with preferential face-to-face alignment (light orange) from those with only weak local order (dark orange). The pie chart (upper left) compares the relative frequency of the 10 observed classes. In each of the classes, polyhedra are listed in decreasing order of the isoperimetric quotient, a measure of the particle's shape. A polyhedron is included multiple times if it was found to assemble into more than one ordered structure. Examples of the various crystal and other structures are shown in upper right. Lower half of figure shows the strong influence of directional entropic "bonding" in the case of non-plastic crystals and liquid crystals, and analogies with traditional materials bonding classes.

Representative Publications

Damasceno, P. F., M. Engel, and S. C. Glotzer. 2012. "Crystalline Assemblies and Densest Packings of a Family of Truncated Tetrahedra and the Role of Directional Entropic Forces." *ACS Nano* 6 (1): 609–614.

Damasceno, P. F., M. Engel, and S. C. Glotzer. 2012. "Predictive Self-Assembly of Polyhedra into Complex Structures." *Science*, 337 (6093): 453–457.

Jankowski, E., and S. C. Glotzer. 2012. "Screening and Designing Patchy Particles for Optimized Self-Assembly Propensity through Assembly Pathway Engineering." *Soft Matter* 8 (10): 2852–2859.

van Anders, G., N. K. Ahmed, R. Smith, M. Engel, and S. C. Glotzer. 2014. "Entropically Patchy Particles: Engineering Valence through Shape Entropy." *ACS Nano* 8 (1): 931–940.

Ye, X., J. Chen, M. Engel, J. A Millan, W. Li, L. Qi, G. Xing, J. E. Collins, C. R. Kagan, J. Li, S. C. Glotzer and C. B. Murray. 2013. "Competition of Shape and Interaction Patchiness for Self-Assembling Nanoplates." *Nature Chemistry* 5 (6):466–473.

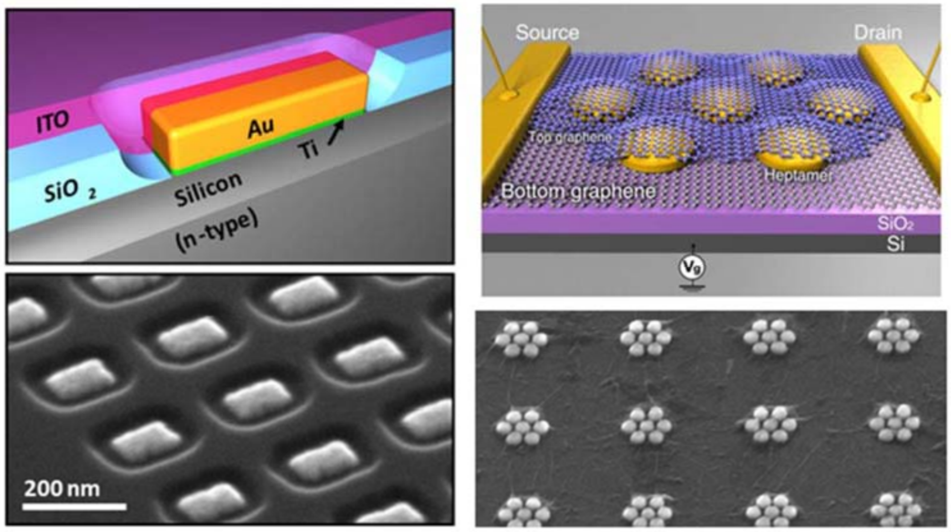
NSSEFF Awardee: Naomi Halas **Year of Award:** 2009

Project Name: 3D Nanophotonics: Bending Light in New Directions

Dr. Naomi J. Halas, the Stanley C. Moore Professor in Electrical and Computer Engineering and a professor in the Physics Department and the Director of the Smalley-Curl Institute at Rice University, was awarded an NSSEFF grant in 2009 to establish a major research program in the nano-engineering of artificial electromagnetic materials at infrared and optical frequencies. The major directions of the research combined theory and multiscale modeling of nanostructures with the design and fabrication of these structures. This project had four goals: (1) Develop photonic materials with entirely new functional behavior based on 3D reduced symmetry metallic nanostructures. (2) Understand, design, and fabricate nano-engineered nonlinear optical materials based on the resonant responses of reduced symmetry nano-structures. (3) Develop new responsive photonic materials based on coherent phenomena to exhibit exotic behavior such as sub-radiance, super-radiance, Fano resonances, and electromagnetically induced transparency. (4) Design and experimentally realize metafluids—liquids or amorphous materials with metamaterials properties independent of polarization or orientation.

Achievements: One of the major accomplishments of this project was the development of a new wavelength-specific light-detection mechanism based on directly combining nanoscale antennas with semiconducting Shottky diode detectors to form a "nano-antenna-diode." Light detection relies on generating "plasmons" in the nano-antennas that decay into hot electrons that are detected as a current by the Shottky diode. The wavelength that is detected is controlled by size of the nano-antennas. The first such device consisted of gold nanostructures on silicon but evolved into a novel graphene-based device where the metallic nanostructures are sandwiched between two sheets of graphene, and the graphene acts as the detector of the hot electrons generated by the nano-antennas (see Figure 15).

A second major accomplishment of this project was the use of similar plasmonic nanostructures to generate large electromagnetic fields that are confined to very small volumes. A metal-capped hemispherical nanoparticle—a "nanocup"—can be used to generate what is known as second harmonic generated (SHG) light. The plasma resonance of the nanoparticle is tuned to the fundamental light frequency. The intensity and the emission direction of the SHG can be modified by the orientation of the nanocup relative to the direction of the incoming light. The up-conversion efficiencies are very large (comparable to current nonlinear optical materials) but provide the capability of accessing regions of the spectrum that are not available to current naturally occurring materials.



Source: Gimm (2013)

Figure 15. Nano-antenna-diode-based Devices: A New Mechanism for Photodetection. Top left: Representation of a single Au resonant antenna on a silicon substrate. Bottom left: Scanning electron micrograph of a representative device array imaged at a 65° tilt angle. Top right: a hybrid plasmonic nano-antenna graphene-based sandwich device. Bottom right: IR nanoantennas sandwiched between two graphene layers of the device.

Representative Publications

Knight, M. W., H. Sobhani, P. Nordlander, and N. J. Halas. 2011. "Photodetection with Active Optical Antennas." *Science* 332, no. 6030: 702–704.

Fang, Z., Z. Liu, Y. Wang, P. M. Ajayan, P. Nordlander, and N. J. Halas. 2012. "Graphene-Antenna Sandwich Photodetector." *Nano Letters* 12, no. 7: 3808–3813.

Zhang, Y., N. K. Grady, C. Ayala-Orozco, and N. J. Halas. 2011. "Three-Dimensional Nanostructures as Highly Efficient Generators of Second Harmonic Light." *Nano Letters* 11, no. 12: 5519–5523.

Fan, J. A., C. Wu, K. Bao, J. Bao, R. Bardhan, N. J. Halas, V. N. Manoharan, P. Nordlander, G. Shvets, F. Capasso. 2010. "Self-Assembled Plasmonic Nanoparticle Clusters." *Science* 328, no. 5982: 1135–1138.

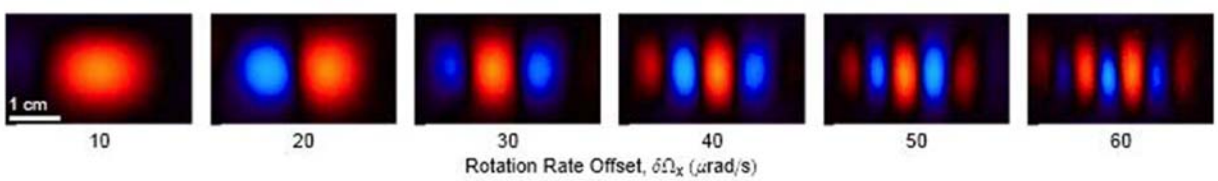
Lassiter, B., H. Sobhani, M. W. Knight, W. S. Mielczarek, P. Nordlander, and N. J. Halas. 2012. "Designing and Deconstructing the Fano Lineshape in Plasmonic Nanoclusters." *Nano Letters* 12, no. 2: 1058–1062.

NSSEFF Awardee: Mark Kasevich **Year of Award:** 2009

Project Name: Atomic de Broglie Wave Navigation Sensors

Dr. Mark Kasevich, Professor of Physics and Applied Physics at Stanford University, was awarded an NSSEFF Fellowship in 2009 to advance the state of the art of atom-interferometry. Quantum mechanics teaches us that there is a particle-wave duality. Light waves can exhibit particle properties (photons), and particles, such as electrons and atoms, can exhibit wave properties, which are known as de Broglie waves, named for Nobel Prize winter Louis De Broglie, who postulated their existence. Kasevich's project involves the interference of these de Broglie matter waves to produce significantly improved inertial force sensors for gravimeters, accelerometers, gyroscopes, and gravity gradiometers. The goal was to realize a thousand-fold improvement over state-of-the-art instruments.

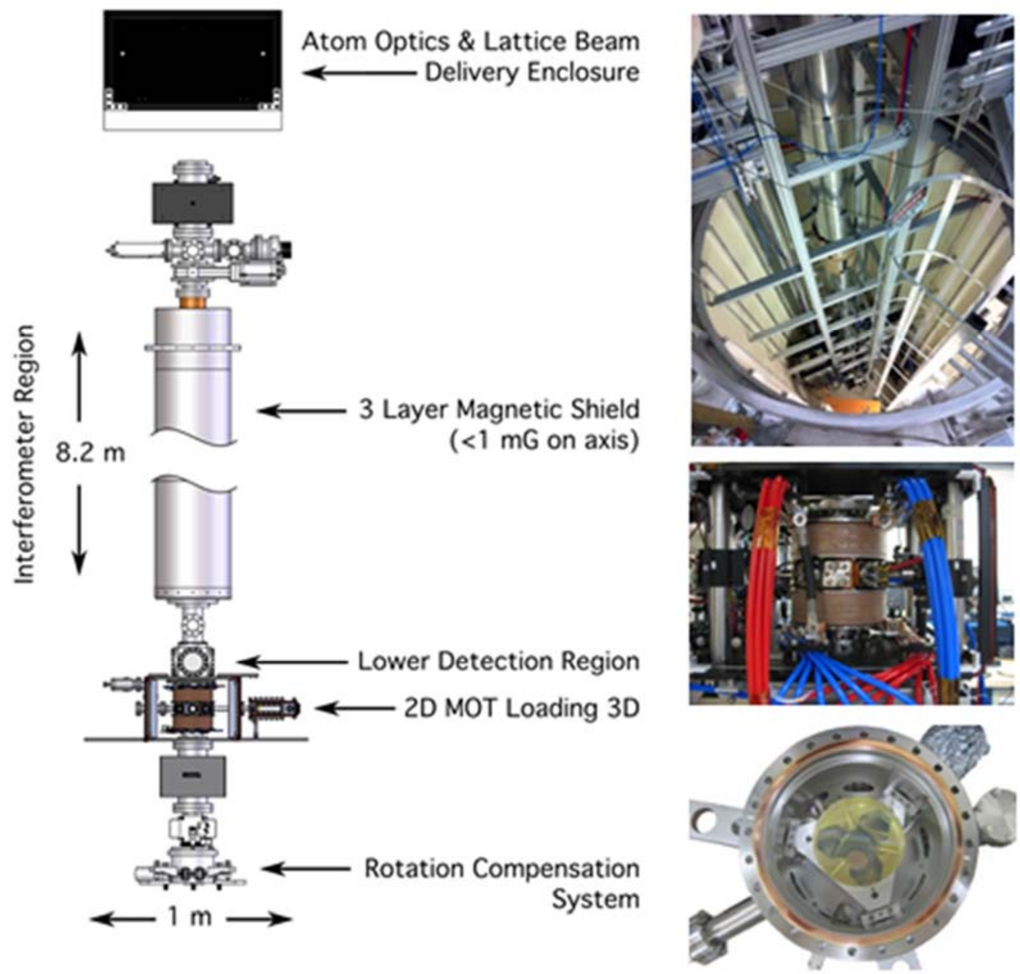
Achievements: This project demonstrated new technologies and methods for atom de Broglie wave interferometry that have indeed enabled orders-of-magnitude improvement over the state-of-the-art methods that existed before this project was initiated. For example, atom interferometric accelerometers achieved an effective noise level of 7×10^{-12} g in a 2.3 sec measurement time, a 500× improvement over previously published work. They also demonstrated new atom optics sensing modalities, including a gyrocompass that achieved 10 millidegree precision in determining true north. An example of the interference fringes produced by atom de Broglie interference is shown in Figure 16.



Source: Gimm (2013).

Figure 16. Images of Interference Fringes Obtained from Interfering Ensembles of Ultra-cold Rb Atoms After Wave Packets Have Been Separated by a Distance of 1.4 cm. Fringe periodicity is determined by the effective rotation rate of the laser beams used to coherently manipulate the atomic wave packets. For these data, atoms were cooled to temperatures of 50 nK and launched on nearly 10 m high ballistic trajectories lasting 2.3 seconds. False coloring denotes the atomic density (blue is low density, red is high density).

To carry out some of these demonstrations Kasevich's team developed a facility that allows for the design and testing of novel, ultra-precision atom interferometric inertial sensing protocols (shown in Figure 17). This facility is based on a 10 m tall evacuated tower that allows more than 2 s of inertial free-fall time. This facility was exploited to demonstrate rotation, acceleration, and gravitational sensing protocols that substantially extended the state of the art. This research has led to additional funding and has initiated a start-up company called AO Sense that is on track to deliver high-performance inertial sensors that have a volume of 1/10 liter at the watt level of power consumption, which is perfect for unmanned autonomous vehicles.



Source: Gimm (2013).

Figure 17. Illustration of the Atom Interferometry Facility. Left: Schematic representation of the apparatus, including, from bottom to top, the precision tip-tilt stage (rotation compensation system), atom source, 8.2 m magnetically shielded interrogation region including the magneto-optic trap (MOT), and the opto-mechanics enclosure for the delivery of the required laser beams. Right: Images of representative subsystems, including the rotation compensation system (bottom), atom source (middle), and magnetically shielded vacuum system (top).

Representative Publications

Chiow, S., T. Kovachy, H.-C Chien, and M. A. Kasevich. 2011. “102$\hbar k$ Large Area Atom Interferometers.” *Physical Review Letters* 107: 130403.

Dickerson, S. M., J. M. Hogan, A. Sugarbaker, D. M. S. Johnson, and M. A. Kasevich. “Multi-Axis Inertial Sensing with long-Time Point Source Atom Interferometry.” 2013. *Physical Review Letters* 111: 083001.

Graham, P. W., J. M. Hogan, M. A. Kasevich, and S. A. Rajendran. 2013. "New Method for Gravitational Wave Detection with Atomic Sensors." *Physical Review Letters* 110: 171102.

Sugarbaker, A., S. M. Dickerson, J. M. Hogan, D. M. S. Johnson, and M. A. Kasevich. 2013. "Enhanced Atom Interferometer Readout through the Application of Phase Shear." *Physical Review Letters* 111: 113002.

Vrijsen, G., O. Hosten, J. Lee, S. Bernon, and M. A. Kasevich. 2011. "Raman Lasing with a Cold Atom Gain Medium in a High-Finesse Optical Cavity." *Physical Review Letters* 107: 063904.

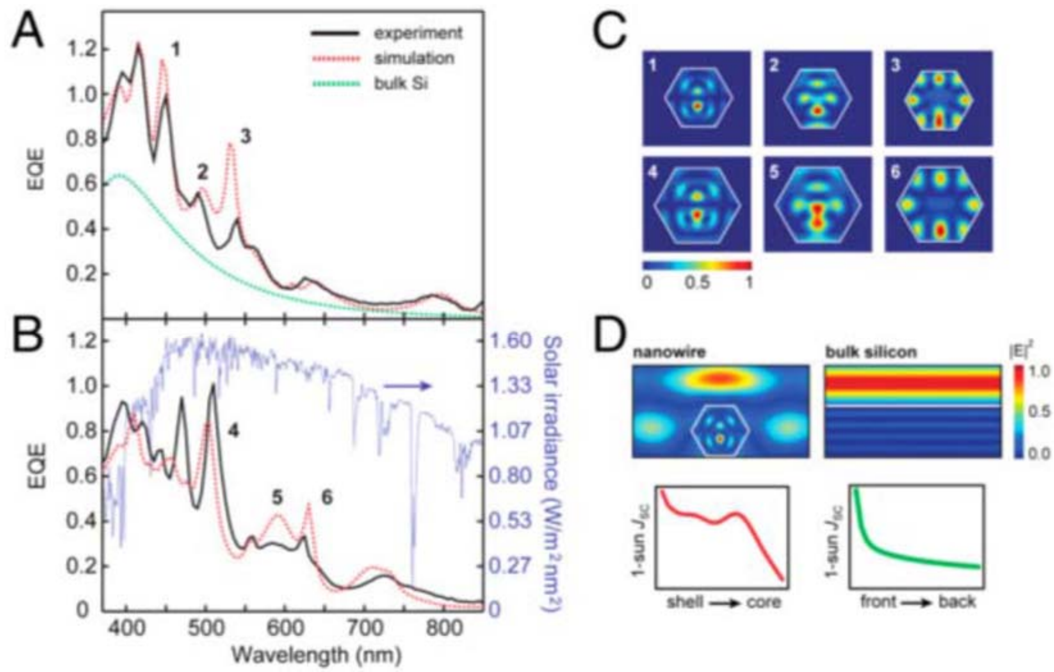
NSSEFF Awardee: Charles M. Lieber **Year of Award:** 2009

Project Name: One-Dimensional Nanostructures as Building Blocks for Functional Electronic and Bioelectronic Materials

Dr. Charles M. Lieber, the Mark Hyman Professor of Chemistry and a professor in John A. Paulson School of Engineering and Applied Sciences at Harvard University, was awarded an NSSEFF fellowship in 2009 to explore the potential of using one-dimensional nanostructures as a broad science and technology platform. These one-dimensional nanostructures, nanowires, are explored as building blocks for functional electronic and bio-electronic materials. Emphasis is on developing efficient nanoscale power sources and ultrasensitive, low-power biocompatible nano-sensors, together with the heterogeneous two- and three-dimensional assembly of these distinct nano-electronic elements to yield self-powered functional electronic nano-systems. The scientific and technical approach involves highly interdisciplinary research focused on (1) the design, synthesis, and structural characterization of nanowire heterostructures with structure/composition variation at the nanometer scale to control specific properties; (2) the fabrication and characterization of nanoscale devices and determining their fundamental electronic properties, power conversion efficiencies, and detection sensitivities; (3) the development of directed assembly strategies capable of multistep transfer of one or more key nanostructures into controlled size and density arrays on rigid and flexible chips; and (4) the design, assembly, heterogeneous integration, and characterization of self-powered nano-systems.

Achievements: Lieber's team has made significant breakthroughs in several distinct areas of this NSSEFF program, including the design, synthesis, and characterization of novel nanowire heterostructures for photovoltaics, the design and development of new nano-electronic bio-probes that can blur the distinction between digital electronics and living matter, and the creation of cyborg tissues. The accomplishments of this team can be divided into three areas: nano-wire-based photovoltaic power elements; novel nano-electronic bio-probes; and cyborg tissues.

Nano-wire-based photovoltaic power elements. Lieber's team has developed synthetic methods to prepare the first radial or coaxial single-crystal nanowire heterostructures with the general structure p-core/i-shell/n-shell, where p, i, and n refer to p-type, intrinsic, and n-type doping, respectively. Specifically, the team completed the synthesis and fabrication of p/n, p/i/n, p/p/n, and p/p/i/n coaxial devices and characterized their photovoltaic properties at the single-nanowire level. These results show clearly that we can synthetically manipulate, in a positive manner, the open-circuit voltage and short-circuit current density via this unique strategy; moreover, analysis of these data demonstrates that the increases in voltage can be attributed to improved interface quality in the coaxial nanostructures. In addition, they have also carried out the first single-nanowire, wavelength-dependent absolute photocurrent measurements. Significantly, these measurements (see Figure 18) reveal size-tunable optical resonances, external quantum efficiencies greater than unity, and current densities double those for silicon films of comparable thickness. In addition, finite-difference time-domain (FDTD) simulations for the measured nanowire structures agree quantitatively with the photocurrent measurements and demonstrate that the optical resonances are due to Fabry-Perot and whispering-gallery cavity modes supported in the high-quality faceted nanostructures (Kempa et al. 2012).

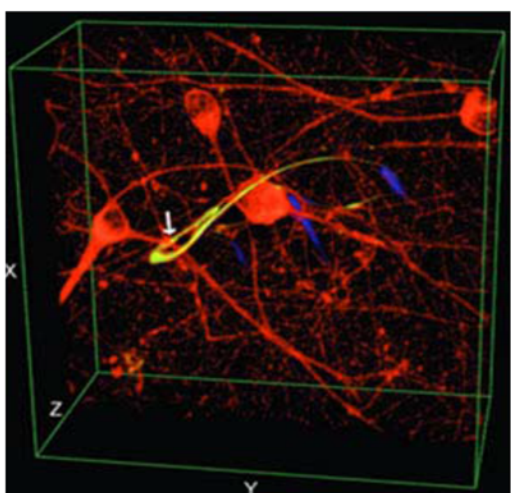


Source: Gimm (2013).

Figure 18. Enhanced and Tunable Absorption in Nanowires (NWs). (A) External quantum efficiency (EQE) as a function of wavelength for a p⁄in NW (black curve) and simulated EQE spectrum (dashed red curve). Dashed green curve shows the simulated spectrum for same thickness of bulk Si. (B) Measured (black curve) and simulated (red curve) EQE spectrum of a p⁄pin NW compared with the irradiance of the AM1.5G solar spectrum (dashed blue curve). (C) FDTD simulations of resonant mode spatial profiles. (D) Electric field intensity for plane wave interacting with a NW (left) and bulk Si (right).

Novel nano-electronic bio-probes. The past three-plus decades of microelectronic and nano-electronic work have focused on planar or two-dimensional (2D) device designs. Such structures have necessitated applications in biology focused on 2D sensing and extracellular recording, despite the inherently three-dimensional (3D) structure of biological systems. Lieber's team has shown that this limitation can be overcome in a general manner through synthetic integration of nanoscale field effect transistor (nano-FET) devices at the tips of hairpin-like kinked nanowires, where nanoscale connections are made by the arms of the kinked nanostructure, and remote multilayer interconnects allow 3D probe presentation. The acute angle probe geometry represents a breakthrough realized by demonstrating the first controlled synthesis of *cis* versus *trans* crystal conformations in any nanomaterial; the nano-FET was localized via modulation doping. 3D nano-FET probes exhibited conductance and sensitivity in aqueous solutions independently of large mechanical deflections and demonstrated high pH sensitivity. In addition, 3D nano-probes modified with phospholipid bilayers can enter a cell with minimal disruption to allow robust recording of the intracellular potentials of living and electrically excitable cells in a highly detailed manner. Specifically, these results confirm that electrical recording arises from the highly localized, point-like nano-FET near the probe tip, which (1) initially records only extracellular potential, (2) simultaneously records both extracellular and intracellular signals as the nano-FET spans the cell membrane, and (3) records only intracellular signals when fully inside the cell. This work was published in *Science* (Tian et al. 2010).

Cyborg tissues. The development of 3D synthetic biomaterials as structural and bioactive scaffolds is central to fields ranging from cellular biophysics to regenerative medicine. Currently, these scaffolds cannot electrically probe the physicochemical and biological micro-environments throughout their 3D and macroporous interior, although this capability could have a marked impact in both electronics and biomaterials. Lieber's team has recently made a major advance by addressing this challenge with the introduction of a new form of electronics; macroporous, flexible, and freestanding nanowire nano-electronic scaffolds (nanoES), and the seamless merger of the nanoES with synthetic or natural biomaterials to create innervated synthetic or cyborg tissues (see Figure 19). 3D macroporous nanoES mimic the structure of natural tissue scaffolds and are formed by self-organization of coplanar reticular networks with built-in strain and by manipulation of 2D mesh matrices. NanoES exhibit robust electronic properties and have been used alone or combined with other biomaterials as biocompatible extracellular scaffolds for the 3D culture of neurons, cardiomyocytes, and smooth muscle cells. In addition, Lieber's team shows the integrated sensory capability of nanoES by real-time monitoring of (1) the local electrical activity within 3D nanoES/cardiomyocyte constructs, (2) the response of 3D nanoES-based neural and cardiac tissue models to drugs, and (3) distinct pH changes inside and outside tubular vascular smooth muscle constructs.



Source: Gimm (2013).

Figure 19. Reconstructed 3D Confocal Microscopy Image of Cyborg Neural Tissue. The colors are as follows: red, rat hippocampal neurons cultured with the nanoES to yield a neural network; yellow and blue, nanoelectronic network; white arrow, neurite passing through ring supporting nanowire transistor.

Representative Publications

Kempa, T. J., J. F. Cahoon, S.-K. Kim, R. W. Day, D. C. Bell, H.-G. Park, and C. M. Lieber. 2012. “Coaxial Multishell Nanowires with High-Quality Electronic Interfaces and Tunable Optical Cavities for Ultrathin Photovoltaics.” *Procedures of the National Academy of Sciences* 109 (5): 1407–1412.

Kim, S-. K., R. W. Day, J. F. Cahoon, T. J. Kempa, K.-D. Song, H.-G Park, and C. M. Lieber. 2012. “Tuning Light Absorption in Core/Shell Silicon Nanowire Photovoltaic Devices Through Morphological Design.” *Nano Letters* 12 (9): 4971–4976.

Tian, B., T. Cohen-Karni, Q. Qing, X. Duan, P. Xie, and C. M. Lieber. 2010. “Three-Dimensional, Flexible Nanoscale Field- Effect Transistors as Localized Bioprobes.” *Science* 329 (5993): 830–834.

Yan, H., H. S. Choe, S. W. Nam, Y. Hu, S. Das, J. F. Klemic, J. C. Ellenbogen, and C. M. Lieber. 2011. “Programmable Nanowire Circuits for Nanoprocessors.” *Nature* 470: 240–244.

Yao, J., H. Yan, and C. M. Lieber. 2013. “A Nanoscale Combing Technique for the Large-Scale Assembly of Highly Aligned Nanowires.” *Nature Nanotechnology* 8:329–335.

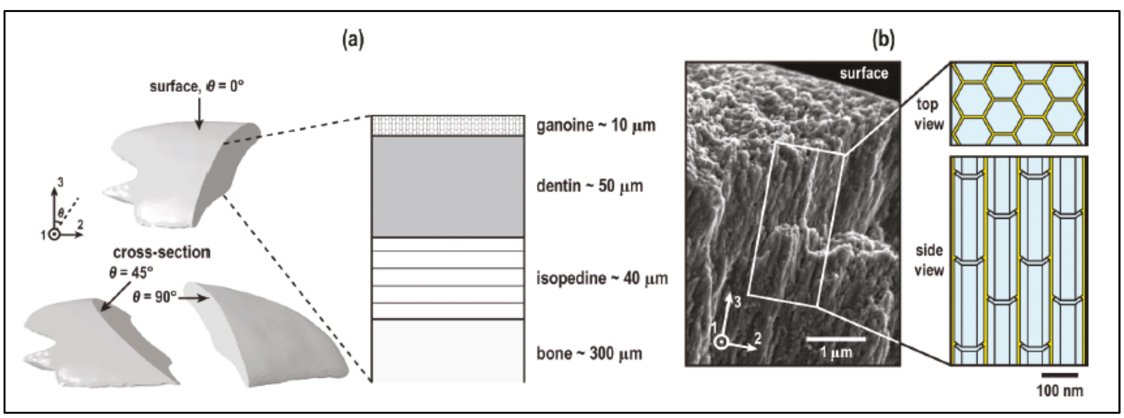
NSSEFF Awardee: Christine Ortiz **Year of Award:** 2009

Project Name: An Untapped Encyclopedia of Engineering Designs for Protective Defense Applications

Dr. Christine Ortiz, the Morris Cohen Professor of Materials Science and Engineering at the Massachusetts Institute of Technology was awarded an NSSEFF fellowship in 2009 to develop a knowledge base of design principles for biologically inspired defense structures of living creatures that could be used to inform new armor and protective materiel designs. The design principles gained through this research may be leveraged to facilitate the development of novel forms of biomimetic materials and structures that may yield new capabilities for protective equipment.

Achievements: The natural systems analyzed covered three categories: (1) articulating/flexible and movable structures, (2) transparent materials, and (3) functional in extreme environments. Ortiz made advancements in each of these areas.

Articulating/flexible structures from nature were analyzed at the microscopic level to identify the molecular structure and how that affected functional capabilities. For example, a scanning electron microscope was used to image (Figure 20) the anisotropic structure of ganoid scales of the polypterus senegalus, sometimes called a dragon fish (Han et al. 2011). By stressing the ganoine layer of the scales from varied angles to determine the range of flexibility or crack propagation of the structure, the team was able to develop a finite-element model that could be provide fundamental design principles. These principles can be used for biomimetic systems like ballistic composite human body armor, where an outermost layer with aligned ceramic or metallic nanocrystals embedded in flexible materials will dissipate energy and deter penetration, but also allow for ample movement.

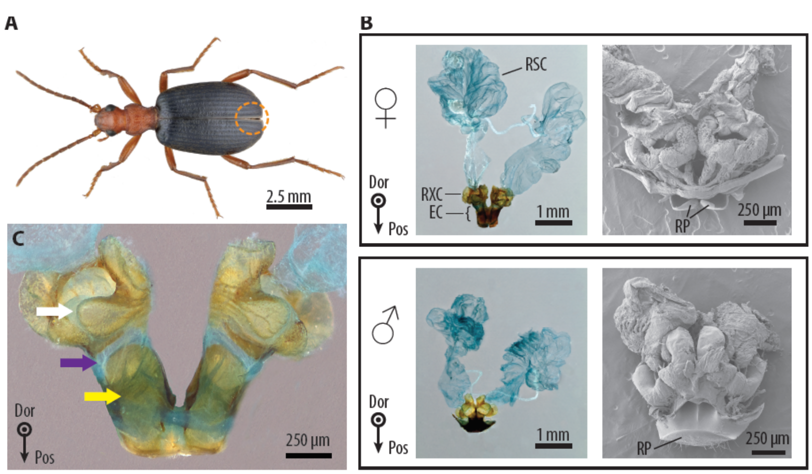


Source: Han et al. (2011).

Figure 20. The Analysis of the Top Layer of a Ganoid Scale to Determine Its Reaction to Physical Insults Applied at Varying Qngles

There are some transparent materials in nature that allow light to pass through but still provide protection from physical insult. For example, the naturally transparent shell in the *Placuna* *placenta*, also known as the windowpane oyster, has a hard but transparent shell that offers the animal physical protection and visual camouflage (Li and Ortiz 2013). In this first of its kind, detailed study of the *P. placenta* that analyzed the optical and mechanical performance at the microstructural level of a natural mineralized transparent structure, Li and Ortiz (2013) used scanning electron and atomic force microscopy to analyze the transparent shell. They found that the shell is composed of laminated layers of calcite that allows for ~85% of light transmission through the shell and, based on the foliated crystal structure interleaved with a thin organic interface, could withstand localized fracturing when stress to a point of failure without radial cracks across the surface that would limit transparency reduction across a surface. The understanding of how the shell provides high optical transparency and mechanical robustness provides design concepts for application of engineering structural transparent materials, like face masks and windshields.

An example of the analyses of living creatures functioning in an extreme environment involved the Bombardier beetles (Brachinini), which are able to produce a hot (~100 °C), pulsed, toxic quinone-based defensive spray through explosions inside their pygidial gland reaction chambers at the rate of approximately 600 Hz (Arndt et al. 2015). Unique to the bombardier beetles is the ability to use an internal explosive chemical reaction to simultaneously synthesize a toxic fluid that is heated and propelled through a forceful spray. High-speed magnified video of the chemical explosions inside living beetles using synchrotron X-ray imaging shows that spray pulsation is controlled by flexible laminated structures located at the junction between the reservoir (reactant) and reaction chambers where the precursor chemicals mix, quickly explode, are exhausted, and reset for the next cycle at a fast pulse rate. The pygidial glands (Figure 21) have a cuticle composite layer of chitin, proteins, and waxes protecting the beetle from the toxic chemicals, heat, and extreme pressure during the explosions. The beetle uses this system as a defense mechanism, spraying potentially harmful threats. This design could be leveraged for novel propulsion mechanisms or active blast mitigation systems.



Source: Gimm (2013).

Figure 21. Bombardier Beetle with Highly Magnified Images of Structures in the Pygdial Glands

Representative Publications

Arndt, E. M., W. Moore, W.-K. Lee, and C. Ortiz. 2015." Mechanistic Origins of Bombardier Beetle (Brachinini) Explosion-Induced Defensive Spray Pulsation." *Science* 348 (6234): 563–567.

Han, L., L. Wang, J. Song, M. C. Boyce, and C. Ortiz. 2011. "Direct Quantification of the Mechanical Anisotropy and Fracture of an Individual Exoskeleton Layer via Uniaxial Compression of Micropillars." *Nano Letters* 11 (9): 3868–3874.

Li, L., and C. Ortiz. 2013. "Biological Design for Simultaneous Optical Transparency and Mechanical Robustness in the shell of *Placuna placenta*." *Advanced Materials* 25 (16): 2344–2350.

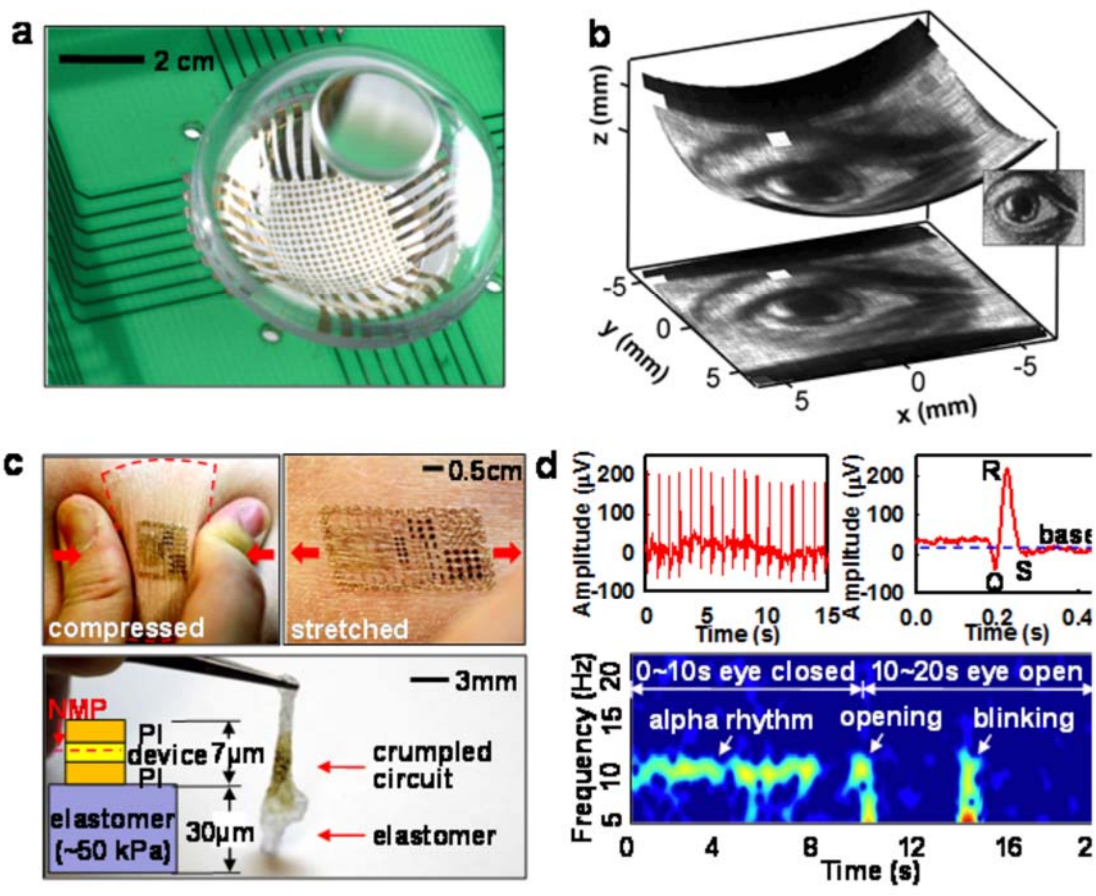
NSSEFF Awardee: John A. Rogers **Year of Award:** 2009

Project Name: Materials and Mechanics for Stretchable Electronics/Optoelectronics

Dr. John A. Rogers, professor from the Department of Materials Science and Engineering at the University of Illinois, Urbana-Champaign and the Director of a Nanoscale Science and Engineering Center, was awarded an NSSEFF Fellowship to develop the basic scientific foundations for a new class of technology—high-performance, mechanically stretchable electronic/optoelectronic systems.

Achievements: The successful strategies that emerged over the course of the research broadly redefine the reach of electronics, from the ultra-flat surfaces of rigid semiconductor wafers to virtually any type of substrate mechanics or shape. Many important applications were demonstrated in areas ranging from intimate integration of electronics with the human body for health monitoring and therapeutic intervention to bio-inspired device designs for wide-field-of-view digital cameras. The topics of the research include (1) semiconductor nanomaterials from single crystalline inorganic (Si, GaAs, GaN and InP) wires, ribbons, and membranes, to single-walled carbon nanotubes, in the form of electronically homogeneous, organized arrays; (2) deterministic assembly schemes that exploit the physics of soft adhesion for controlled manipulation of these nanomaterials; and (3) mechanics and structural design in hybrid systems consisting of ultrathin layers of rigid materials intimately coupled to elastomers, to achieve overall architectures that provide high elongation and low effective modulus. The collective scientific outcomes establish a proven route to semiconductor devices and systems with performance comparable to those of state-of-the-art wafer-based technologies, but with the mechanics of a rubber band. These results are now in initial stages of commercialization in health/wellness products and advanced surgical tools.

This project has had several recent key results that established a base of scientific understanding on essential aspects of materials, mechanics principles, and integration techniques for high-performance electronic/optoelectronic devices. This understanding helped create materials that exhibit linear elastic responses to large strain (~100%) deformations. The technologies resulting from these materials created new opportunities for integrating electronics with the soft tissues of the human body and for exploiting biologically inspired device designs. The research involves three main areas: (1) semiconductor nanomaterials, in shape-engineered forms, as the active components; (2) strategies to assemble these materials into desired layouts on substrates of interest; and (3) circuit/device designs that minimize strains in these and other "hard" constituent materials when integrated on "soft" elastomers. Interconnected assemblies of nanomaterials can be exploited to form stretchable electronic/optoelectronic devices. Here, analytical and computational mechanics models define layouts that minimize strains in the semiconductors and other electronic materials, most of which fracture at strains of only ~1%, or less. As testbed applications, they focused on two classes of technology that are not addressable by any existing form of electronics: (1) digital cameras with bio-inspired, hemispherical layouts and (2) bio-integrated devices for clinical use in cardiology, neurology and other related areas of medicine. Figure 22a shows an electronic "eyeball" camera that incorporates a hemispherically curved photodetector array with the size and shape of the human eye. The fabrication begins with the formation of a planar, interconnected array of silicon photodiodes in a mesh geometry. Controlled compressive deformation using a shaped, thin elastomer stamp accomplishes a planar-to-hemispherical geometry transformation and transfer to the concave surface of a glass support. Coupling a simple plano-convex lens fixed in a transparent hemispherical shell completes the camera. The fields of view, levels of aberration, and illumination uniformity that are possible with this hemispherical design all exceed those achievable with conventional flat photodetector arrays when similarly simple optics are used. Figure 22b presents a picture captured with this camera, rendered in the hemispherical geometry of the detector (top) and as a planar projection (bottom); the actual object appears in the right inset.



Source: D. H. Kim et al., 2011a.

Figure 22. Images of an Electronic Eyeball Camera (a) and Skin-mounted Electronics (c), with Representative Data Collected from each (b, d)

As an example of bio-integration, electronics can be configured with physical properties, ranging from modulus to degree of stretchability, areal mass density, thickness, and flexural rigidity, that precisely match those of the epidermis. Such devices laminate directly onto the surface of the skin, much like a temporary-transfer tattoo, to provide various types of health-care and non-health-care-related functions. An image of a demonstration platform appears in Figure 22c; the structure includes antennas, wireless power coils, silicon nano-membrane transistors and diodes, strain and temperature gauges, along with radio frequency inductors, capacitors, and oscillators. Figure 22d presents measurement results for electrocardiography (ECG, top) and electroencephalography (EEG, bottom) recorded with epidermal electronic systems mounted on the chest and forehead, respectively. The ECG measurements show clear QRS signatures; the EEG traces exhibit characteristic alpha rhythms when the subject's eyes are closed. Many other possible devices, ranging from acute implants to surgical tools, can also be realized.

Representative Publications

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Kim, D.-H., N. Lu, R. Ma, Y.-S. Kim, R.-H. Kim, S. Wang, J. Wu, S. M. Won, H. Tao, A. Islam, K. J. Yu, T. Kim, R. Chosdhury, M. Ying, L. Xu, M. Li, H Chung, H. Keum, M. McCormick, P. Liu, Y. Zhang, F. G. Omenetto, Y. Huang, T. Coleman, and J. A Rogers. 2011a. "Epidermal Electronics." *Science* 333, no. 6044: 838–843.

Kim, D.-H., N. Lu, R. Ghaffari, Y.-S. Kim, S. P. Lee, L. Xu, J. Wu, R.-H Kim, J. Song, Z. Liu, , J. Viventi, B. de Graff, B. Elolampi, M. Mansour, M. J. Slepian, S. Hwang, J. D. Moss, S. Won, Y. Huang, B. Litt, and J. A. Rogers. 2011b. "Materials for Multifunctional Balloon Catheters with Capabilities in Cardiac Electrophysiological Mapping and Ablation Therapy." *Nature Materials* 10, no. 4: 316–323.

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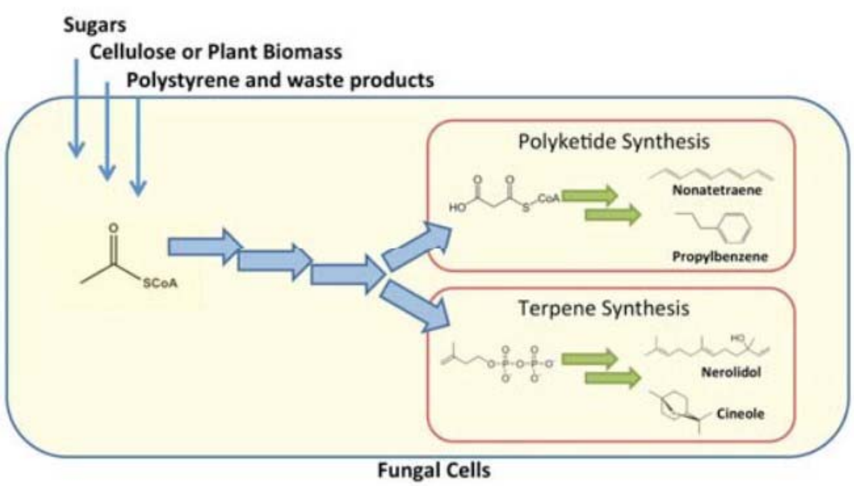
NSSEFF Awardee: Scott Strobel **Year of Award:** 2009

Project Name: Exploitation of Diesel Producing Fungi as a Renewable Source of Fuel

Dr. Scott A. Strobel, the Henry Ford II Professor in the Molecular Biophysics and Biochemistry Department at Yale University, was awarded an NSSEFF fellowship in 2009 to develop emerging biotechnology to facilitate the development of using fungi to produce hydrocarbons that can function as transportation fuels from cellulose or other readily available alternative sources. The Department of Defense uses tremendous amounts of fuel and would benefit greatly from a method that could produce fuel for jets, trucks, and tanks that is not reliant on fossil fuels.

Achievements: Strobel identified multiple fungi that produce hydrocarbons that could potentially be used as fuel. To produce fuel compounds, fungi ingest an energy source (e.g., sugar, cellulous, or other waste products) and produce hydrocarbons (see Figure 23). The type of hydrocarbon produced and the rate at which this is done are determined by the genetic makeup of the fungus used, the type of energy source used as food for the fungus, and environmental particulars (i.e., growth medium) where the process takes place. Strobel's research has focused on optimizing genetic sequencing techniques to identify genotype and phenotype specifics to more quickly address validation and scaling issues. These efforts rely on high-throughput genetic sequencing and heterologous expression in model organisms, along with detecting hydrocarbon production within a culture, to determine if the output has properties that make it a good surrogate for a transportation fuel.



Source: Gimm (2013).

Figure 23. The Fungi Ingest an Energy Source (e.g., sugar, cellulous, or other waste products) and Convert them to Compounds that can be Used as Transportation Fuels

Some biofuels in the past have used human food sources such as corn, soybeans, and sugarcane as feedstock, which has led to some concern that the production of biofuels may subsequently raise food costs. This was one of the suggested reasons that contributed to a worldwide food shortage in 2008 (Mitchell 2008). Because the fungi and processes examined by Strobel would use nonfood sources, there is no competition for food sources, which can drive up prices. In addition, one of the potential feedstocks is consumer plastic waste, so the process may also decrease the consumer waste problem. Other potential sources include cellulosic biomass, which includes nonedible portions of plants (Gianoulis et al. 2012).

Strobel's focus has been on fungal endophytes, organisms that live within some plants and are symbiotic with their host plant (Shaw et al. 2015). Some of the promising fungi studied by Strobel are listed in Table 1 (Shaw et al. 2015). Each of the fungi has genetic variants, and one of the key components of Strobel's research is to understand the genetic basis that may make particular organisms of specific variants better/worse at producing fuel compounds.

Table 1. Some of the Promising Fungi Studied by Strobel

Organism	Fuel Produced
Ascocoryne sarcoides NRRL50072	C6–C9 alkanes (like octane), alcohols, aldehydes, and other molecules similar to those found in gasoline
Pleosporales spp. E5202H and E8604B	Polyene, a potential gasoline surrogate
Nodulisporium sp. E7406B	Terpene cineole, a potential jet fuel surrogate
Phomopsis *sp.* BR109A	Monoterpenes and sesquiterpenes (potential jet fuel surrogates) and diterpene (potential marine diesel surrogate)
Pestalotiopsis microspora E2712A	Degrades plastic to produce medium chain alcohols
Musocodor albus CZ-620	Medium-chain alcohols and esters

This type of research requires extensive exploration for minute organisms that live in and on certain plants in remote locations like rainforests (Forcina et al. 2015). The process entails finding and gathering many potential samples and bringing them back to the lab for analysis and testing. Some of these organisms have been found in foreign countries that may consider a specific fungus a national resource, which may limit their export and commercial use. Understanding the genomic requirements and bio-synthesizing process of these fungi at a fundamental level is therefore an important step in identifying new, more easily obtainable fungi or in genetically modifying the properties of existing available fungi to produce fuels in a commercially viable manner (Spakowicz and Strobel 2015).

Representative Publications

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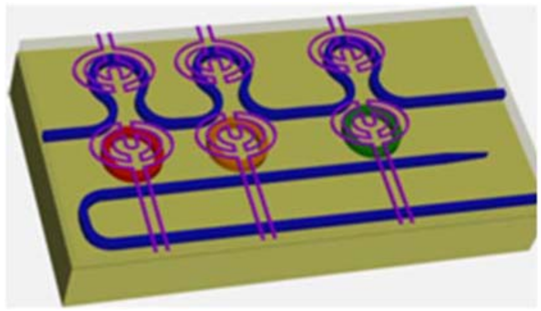
NSSEFF Awardee: Andrew M. Weiner **Year of Award:** 2009

Project Name: Novel Ultraband Photonic and Radio-Frequency Systems for Communications, Sensing and Countermeasures

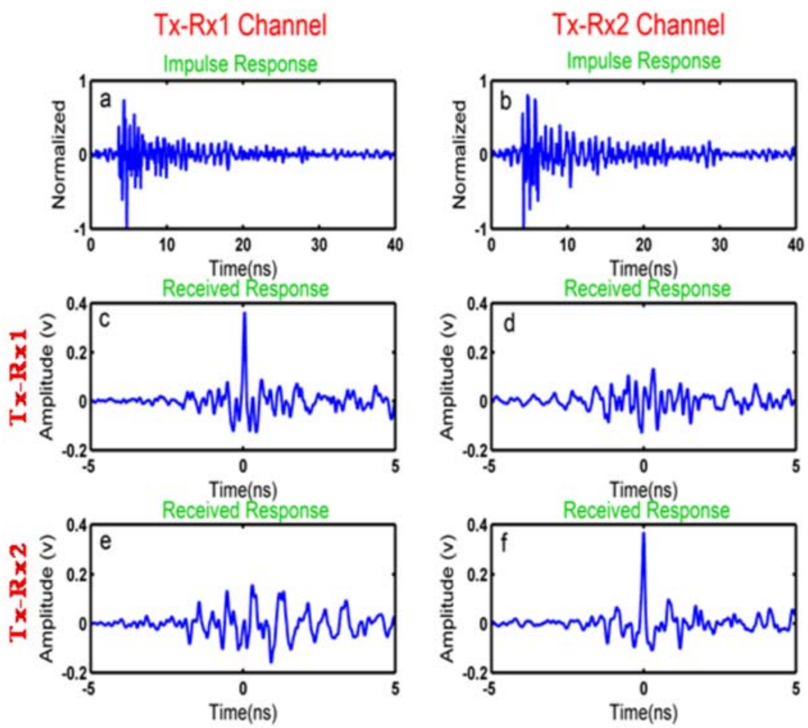
Dr. Andrew M. Weiner, the Scifres Family Distinguished Professor of Electrical and Computer Engineering at Purdue University, was awarded an NSSEFF fellowship in 2009 to explore unique aspects of RF technology as applied to systems such as radar, sensing, wireless communications, and electronic warfare that are vital to national security. Conventional RF systems are usually designed to operate at low instantaneous bandwidth, with signals possessing a well-defined (though perhaps slowly tunable) frequency. Coherent, phase-based signaling schemes are employed, but only within a narrow instantaneous frequency band. On the other hand, optical systems can be extremely broadband, generating pulses with durations down to femtoseconds, and with terahertz instantaneous bandwidths. Such ultrashort-pulse optical systems are fundamentally time-domain in nature, and phase control over the full bandwidth is crucial. For their NSSEFF program, they have aimed to adapt approaches already proven in the field of broadband optics to pursue new opportunities in generation, processing, and application of ultra-broadband RF electrical signals. The resulting hybrid photonic-RF approach studies have led to new possibilities for manipulation of signals in both RF and photonic domains.

Achievements: Weiner's team has made significant technological advances that are in primarily four areas. (1) Using photonic approaches they have generated user designed RF waveforms that for the first time can fill the RF W band (~75–110 GHz) and have shown through laboratory experiments that these signals hold promise for very high spatial resolution radar imaging. This hybrid approach is schematically shown in Figure 24, which illustrates a photonic RF arbitrary waveform generator. (2) The team has also demonstrated, for the first time, that electro-optic modulator technologies can be harnessed for temporal cloaking at telecommunications rates. Their apparatus controls the flow of light such that temporal holes are opened and closed billions of times a second, rendering signals that occur during the temporal holes undetected. This work, reported in the prestigious journal *Nature*, may have implications for secure and tamper-free lightwave communications. (3) Nonlinear optical effects in chip-scale optical micro-resonators allow for conversion of a single laser frequency into optical frequency combs comprising dozens, or even hundreds, of equally spaced optical frequencies. Such chip-scale devices offer the potential to take frequency combs out of the research laboratory and into practical applications. Similar devices have been previously demonstrated with relatively large mode-locked lasers, which had enormous impact (e.g., the 2005 Nobel Prize in Physics). The team's work on such chip-scale frequency combs has resulted in follow-up funding from DARPA, AFOSR, and NSF to address further photonic integration issues, to provide additional scientific understanding, and to investigate applications in RF signal processing and telecommunications. (4) Under NSSEFF the team advanced the state of the art on precise measurement and control of broadband RF signals propagating in complex indoor wireless environments. This process in the presence of multipath interference in an indoor environment is illustrated in Figure 25. Based on some of this work, the team is contributing to a DARPA study focused on ultra-broadband RF signaling for jamming-resistant, assured communications for ground-air communications links.



Source: Gimm (2013).

Figure 24. Silicon Photonic Spectral Shaper Chip for Photonic RF Arbitrary Waveform Generation. The spectrum of a broadband input pulse from a mode-locked laser (not shown) is shaped via interaction with eight cascaded microring resonators. Through thermo-optic tuning and interferometric couplers, both the amplitude and frequency of the various resonances can be programmed independently, leading to substantial flexibility for arbitrary waveform generation.



Source: Gimm (2013).

Figure 25. Compensation of Ultra-broadband Multipath Distortion via Photonics-enabled RF Waveform Generation. A 2–18 GHz transmit antenna (Tx) sends RF signals to a pair of closely spaced receive antennas (Rx1, Rx2) in an adjacent room. (a), (b) Impulse responses measured between Tx and Rx1/Rx2 antennas. (c) ,(d) Tx waveform set to compensate Tx-Rx1 path, achieving compression to a strong peak. Rx2 signal remains noiselike. (e), (f) Tx waveform set to compensate Tx-Rx2 path, achieving compression at Rx2; Rx1 signal remains noiselike. Such spatially selective peaking offers potential for covert communications and increased data rate.

Representative Publications

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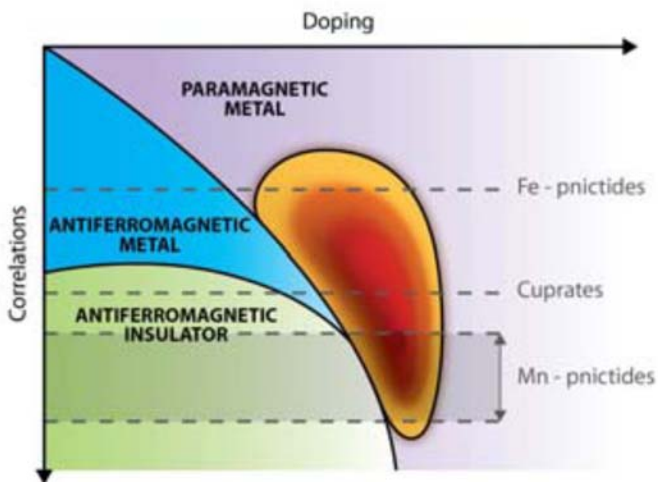
NSSEFF Awardee: Meigan Aronson **Year of Award:** 2010

Project Name: Designing New Higher Temperature Superconductors

Dr. Meigan Aronson, a professor in the Department of Physics and Astronomy at the State University of New York at Stony Brook and a researcher in the Condensed Matter Physics and Materials Science Department at Brookhaven Lab, was awarded an NSSEFF fellowship in 2010 to integrate electronic structure calculations with the synthesis of new superconducting materials, with the aim of providing a rigorous test of the apparent association of high-temperature superconductivity with electron delocalization transitions occurring at quantum critical points. This general idea is illustrated in Figure 26, which shows a generic phase diagram for strongly correlated materials.



Source: Gimm (2013).

Figure 26. A Schematic Phase Diagram for Compounds with Different Strengths of Correlations and Differing Degrees of Charge Doping. Compounds with strong correlations like the cuprates are insulating until doping drives them metallic. Weakly correlated compounds like the Fe-pnictides are always metallic, although doping destroys magnetic order. Superconductivity is nestled in the confluence of the metal-insulator transition and the destabilization of magnetic order. Mn pnictides such as LaMnPO may be more strongly correlated than the cuprates, potentially leading to larger values of Tc although this has not yet been realized.

Achievements: This was an unusual award since it consisted of a collaboration with a team of world-class scientists, each assigned a role in integrating theory with experiment. The senior members of this collaboration were Meigan Aronson and Dimitri Basov (University of California, San Diego); Gabriel Kotliar, Martha Greenblatt, and Girsh Blumberg (Rutgers University); James Allen (University of Michigan); Liu Hao Tjeng (Max Planck Institute for Chemical Physics, Dresden); Stephen Julian (U. Toronto); and Liling Sun and Zhongxian Zhou (Chinese Academy of Sciences, Institute of Physics, Beijing). The team used realistic electronic structure calculations to assess which transition metal monopnictides are closest to electron delocalization and hence optimal for superconductivity. As in the pnictides, the calculations started with a functional layer that is matched with a layered host taken from an extensive library of known framework structures, candidate materials with the appropriate electronic structure were identified and then single crystals were synthesized. Rapid turnaround characterization determined the basic properties of these new materials, identifying the most promising candidates. Optical conductivity and angle-resolved photoemission measurements were used to compare the actual electronic structure with theoretical results, providing feedback to the initial choices of functional and charge reservoir layers.

This team developed a new methodology—"theory-assisted synthesis"—as a means to design and then synthesize new materials with specific functionalities. The goal of this project was to develop a new family of compounds with high superconducting transition temperatures, but this approach should also be applicable to different functionalities like thermoelectricity, insulating gap instabilities, and perhaps magnetic order. A collaborative approach was required to carry out this project, where the group PI Meigan Aronson was responsible for synthesizing new materials and assessing their basic properties. An enabling step was that electronic structure calculations are only now becoming accurate enough to be predictive. Prof. Gabriel Kotliar's group carried out dynamical mean field theory (DMFT) calculations of the electronic structure, providing not only accurate determinations of the electronic structure in these inherently highly correlated materials but also explicit results for the photoemission and optical conductivity that can be directly compared to experimental results. The group of Prof. Dimitri Basov (University of California San Diego) performs optical spectroscopy experiments, which are ideal for distinguishing between metals and insulators, and which, in combination with DMFT, can determine the overall strength of the electronic correlations. Prof. Hao Tjeng's group (Max Planck Institute for Chemical Physics, Dresden) provides information about the transition metal valence state via X-ray absorption, and as well photoemission measurements that can be directly compared to theoretical results from Kotliar's group. Finally, the group of Dr. Liling Sun and Zhongxian Zhou (Chinese Academy of Sciences, Institute of Physics, National Laboratory on Superconductivity) carry out X-ray diffraction measurements and X-ray absorption measurements under high pressures, as well as high-pressure resistivity and magnetic susceptibility measurements, which are inputs needed for the DMFT to calculate idealized lattice constants for transforming insulators to metals.

The initial test of this methodology was to determine if Mn-based compounds (there were none previous to this work) isostructural to the parent Fe-based pnictide superconductor could be driven metallic by doping or pressure, and then potentially superconducting. The system chosen for study was the LaMnPO compound. Optical measurements found that the 1 eV insulating gap in LaMnPO is in excellent agreement with the DMFT predictions, as is the ordered Mn moment determined from neutron-diffraction experiments. Indications of incipient charge delocalization were found in the computed electronic states, also evident in X-ray absorption measurements. Encouraged by this agreement, the researchers explored different doping vectors but were never able to transform LaMnPO into a bona fide metal. They turned next to high pressure and here met success. The electrical resistivity of LaMnPO, evolves from strongly insulating to metallic above ~12 GPa of hydrostatic pressure. Using atomic positions derived from high-pressure X-ray diffraction measurements, it was possible to determine the pressure dependence of the insulating gap, which was found to vanish at ~10 GPa. Intriguingly, the calculations indicate that the Mn moment does not collapse at the insulator-metal transition and that an intermediate metallic phase with magnetic order is produced. Only at pressures higher than 30 GPa is the magnetism fully suppressed. This prediction was subsequently tested with high-pressure magnetic susceptibility measurements, which found that the antiferromagnetic order vanishes in LaMnPO at 30 GPa These experiments show that the conditions under which superconductivity may occur are more diverse than was generally believed. The excellent quantitative agreement between theory and experiment that was found in LaMnPO proved that theory-assisted synthesis is potentially feasible. Unfortunately, no superconductivity was found in pressurized LaMnPO, at least not above ~10 K.

A second goal was adopted for the collaboration, which was to use this approach to find Mn-based superconductors. The LaMnPO measurements indicate that Mn-based compounds can have the same range of behaviors as are found in successful superconductors like the cuprates and the Fe-based superconductors. Here the challenge is to produce a simultaneous collapse of the insulating gap and the magnetic moments, either as functions of pressure or doping. However, the calculated electronic structure of LaMnPO has been used as the template for a larger family of compounds with different Mn-Mn spacings and different Mn coordinations. These calculations were used to form a phase diagram with magnetic insulator, magnetic metal, and nonmagnetic metal (most likely to be superconducting) phases, represented as functions of Mn spacings and angles. This first application of the predictive mode of theory-assisted synthesis has narrowed down the range of desired materials attributes from hundreds of possible compounds in the crystal structure databases to only a few. Very recently superconductivity was found in the first Mn-based compound, MnP at high pressure. The emergence of superconductivity at a quantum critical point where magnetic order disappears was a definite prediction of this project and should lead to the discovery of additional superconductors.

Representative Publications

Guo, J., J. W. Simonson, L. Sun, Q. Wu, P. Gao, C. Zhang, D. Gu, G. Kotliar, M. Aronson, and Z. Zhao. 2013. “Observation of Antiferromagnetic Order Collapse in the Pressurized Insulator LaMnPO.” *Scientific Reports* 3, Article No. 2555.

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NSSEFF Awardee: Alper Atamturk **Year of Award:** 2010

Project Name: Optimal Design of Resilient Capacitated Networks

Dr. Alper Atamturk, professor from the Department of Industrial Engineering and Operations Research at the University of California, Berkeley, was awarded an NSSEFF Fellowship in 2010. This award was focused on providing answers to questions related to defending our national infrastructure networks against random failures and malicious coordinated attacks by adversaries and ensuring the resilience of these networks. Ensuring this resilience is one of the highest priorities of the government. Many of these networks are physical (e.g., oil and gas storage and pipelines, computer networks, power plants and grids). Others, however, such as military logistics and information chains, are logical networks with components of other physical and/or logical networks (e.g., internet, factories, warehouses, ports, satellites, and various modes of transportation and communication channels).

Examples of questions Atamturk investigated in the current research project are as follows:

- If capacities of the components of a network are random variables, what is the optimal (least cost) network configuration that guarantees transshipment of a certain percentage of the traffic between sources and targets with a desired probability?
- What is the optimal (least cost) network configuration that guarantees transhipment of a certain percentage of the traffic between sources and targets when a network is under coordinated attack by an adversary with resource constraints?

Answers to such questions are not only useful for identifying critical vulnerabilities of our infrastructure networks, but also for efficient allocation of scarce resources to mitigate the effects of those vulnerabilities. Furthermore, they can be used to quantify the trade-off between the cost of investment and resilience of our networks for informed decision-making. At the same time, efficient allocation of assets and resources is a major concern with respect to the effectiveness of the surveillance, reconnaissance, and interdiction of terrorist and drug networks. It turns out that the problem of optimal persistent interdiction of an enemy network against an adversary who can shore up the links, or when link capacities are probabilistic, is the duel of optimal resilient network design problems. An interdiction is persistent if it disrupts the enemy traffic to a large extent when the enemy network capacities are uncertain. This project developed novel methods for quantitative analysis of the trade-off between the cost and effectiveness of interdiction.

Achievements: Atamturk and his team solved the very difficult problem of performing an optimization over probabilistic constraints on cuts of a network. The challenge was to identify the right set of a small number of constraints to perform the optimization over, as it is practically impossible to include all the many constraints. The task required decomposing the overall optimization problem into two subproblems: (1) a relaxed problem with fewer constraints and (2) a separation problem to identify missing constraints for the relaxed problem. Both these problems are still nonlinear-integer-optimization problems, but practically easier to solve than the overall problem. Using them iteratively could potentially lead to efficient solutions, even though the team's initial attempts were not computationally viable as many hours of computing were required even for small instances. Through better understanding of the structure of the problems and tangent hyperplane approximations, the team made major breakthroughs in modeling both problems in a convenient way and solving them in a manner of minutes.

Representative Publications

Ahmed, S., and A. Atamtürk. 2011. "Maximizing a Class of Submodular Utility Functions." *Mathematical Programming* 128, no. 1: 149–169.

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Atamtürk, A, and V. Narayanan. 2011. "Lifting for Conic Mixed-Integer Programming." *Mathematical Programming* 126, no. 2: 351–363.

Atamtürk, A., G. Berenguer, and Z.-J. Shen. 2012. "A Conic Integer Programming Approach to Stochastic Joint Location-Inventory Problems." *Operations Research* 60, no. 2: 366–381.

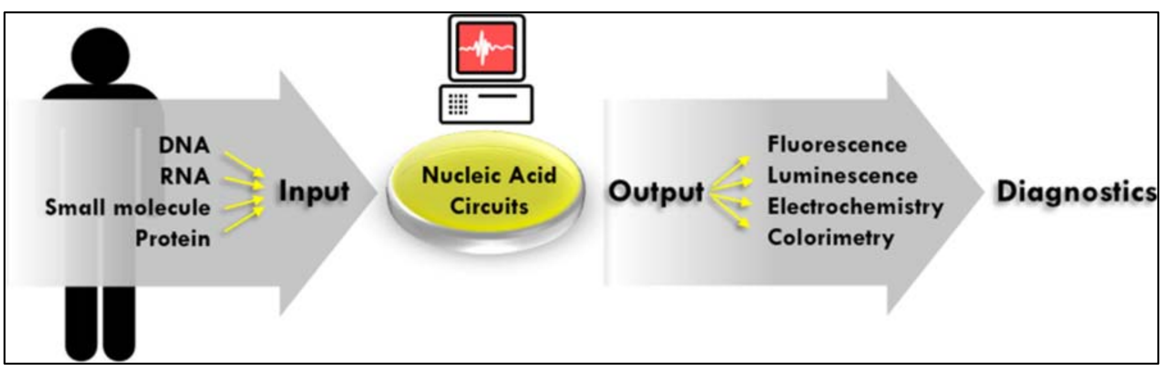
Atamtürk, A., L. F. Muller, and D. Pisinger. 2012. "Separation and Extension of Cover Inequalities for Conic Quadratic Knapsack Constraints with Generalized Upper Bounds." *INFORMS Journal on Computing* 25, no. 3: 420–431.

NSSEFF Awardee: Andrew Ellington **Year of Award:** 2010

Project Name: Developing Biological Software via Genetically Augmented Proteins

Dr. Andrew Ellington, the Fraser Professor of Biochemistry at the University of Texas at Austin, was awarded an NSSEFF grant in 2010 to study how to adapt biology for developing programmable organisms that can be engineered for particular functions and applications. In synthetic biology, there is the basic notion that there are component biological "parts" that can be used as "synthetic circuits" whose function is modular, predictable, and extendable. This is similar to how electronic components like transistors, resistors, and capacitors can be used together on a silicon wafer to form an integrated circuit. Ellington's research has addressed the standardization of the programmable components and the underlying logic for their use to create programmable molecules, such as DNA, and systems that are a new type of genetic software.

Achievements: New methods found by Ellington's team highlight the potential impacts of DNA circuitry on DNA nanotechnology and provide new tools for further development of these fields (Li, Jian, Chen, and Ellington 2012; Jung, Allen, and Ellington 2016). One such method is the use of catalyzed hairpin assembly (CHA) as a signal-amplification reaction. CHA can be used to analyze the spatial structure of DNA through the detection of toeholds (i.e., inserting new information along a compatible strand) and branch migrations (i.e., similar pairs of DNA strands are dynamically joined along the sequence) in proximity that catalyze the CHA reaction. By applying this method to sensing reorganization during the DNA self-assembly processes (i.e., hybridization), the team showed CHA circuits could detect certain hybridization defects, which allowed for the development of a "signal-on" assay that responds to mutations in DNA strands. This is of great interest in genotyping and molecular diagnostics and bio-sensing, as well as for constructing DNA nanotechnology. This research helps set the foundation for tools to analyze DNA sequence and structure that could be used in genetic computing and medical diagnostics.



Source: Image from Jung and Ellington (2014).

Figure 27. A Promising Use of DNA Circuits is for Medical Diagnostics, but They May also be Used for a Broad Range of Other Purposes

Ellington and his team have built multiple novel DNA circuits to demonstrate some of the possibilities of biological software. One example involves the use of DNA molecules as sensors that react to diffuse light to detect the edges of an image; it is the first demonstration of a programmable pattern-transformation mechanism using DNA circuits (Chirieleison et al. 2013). Because these circuits can be made compactly (approximately 1 micron in length) such mechanisms paired with other complex DNA circuits may produce novel functions in bioengineering.

To develop and isolate particular DNA sequences new methods to manipulate have been developed by Ellington and his team. One of those new techniques is the use of emulsions as a method that can overcome some of the barriers for using live bacteria, like *E. coli,* that require the bacteria to stay alive while producing the genetically determined proteins (Lu and Ellington 2013). With emulsions, little compartments can be formed that encapsulate the DNA material being used to keep it isolated from the surrounding environment. Because the emulsions can be made with nonliving compounds they have a much broader range of response to environmental conditions (e.g., temperature, pH levels). By using an emulsion, the effort to identify, select, and apply the templates that generate the most positive results is done relatively easily by breaking the emulsion.

In addition to developing new methods for creating DNA circuits, Ellington is also working to catalog and characterize the different ways that DNA circuits can function (Jung and Elllington 2014). Ellington and his collaborators are developing mathematical models on how to dynamically manipulate the system or allow the system to self-regulate through biological feedback mechanisms (Enyeart, Simpson, and Ellington 2015). These advances will facilitate the development of increasingly more complicated circuits that may lead to improved medical diagnostic/treatment methods and environmental sensing. Ellington is continuing this work for DoD through contracts with DARPA, AFOSR, and ONR.

Representative Publications

Allen, P. B., S. A Arshad, B. Li, X. Chen, and A. D. Ellington. 2012. “DNA Circuits as Amplifiers for the Detection of Nucleic Acids on a Paperfluidic Platform.” *Lab on a Chip* 12 (16), 2951–2958.

Chirieleison, S. M., P. B. Allen, Z. B Simpson, A. D. Ellington, and X. Chen. 2013. “Pattern Transformation with DNA Circuits.” *Nature Chemistry* 5 (12): 1000–1005.

Enyeart, P. J., Z. B. Simpson, and A. D. Ellington. 2015. “A Microbial Model of Economic Trading and Comparative Advantage.” *Journal of Theoretical Biology* 364*:*326–343.

Jung, C., and A. D. Ellington. 2014. “Diagnostic Applications of Nucleic Acid Circuits.” *Accounts of Chemical Research* 47 (6): 1825–1835.

Jung, C., P. B. Allen, and A. D Ellington. 2016. “A Stochastic DNA Walker That Traverses a Microparticle Surface.” *Nature Nanotechnology* 11 (2): 157–163.

Li, B., Y. Jiang, X. Chen, and A. D. Ellington. 2012. “Probing Spatial Organization of DNA Strands Using Enzyme-Free Hairpin Assembly Circuits.” *Journal of the American Chemical Society* 134 (34): 13918–13921.

Lu, W.-C., and A. D. Ellington. 2013. “In Vitro Selection of Proteins via Emulsion Compartments.” *Methods* 60 (1): 75–80.

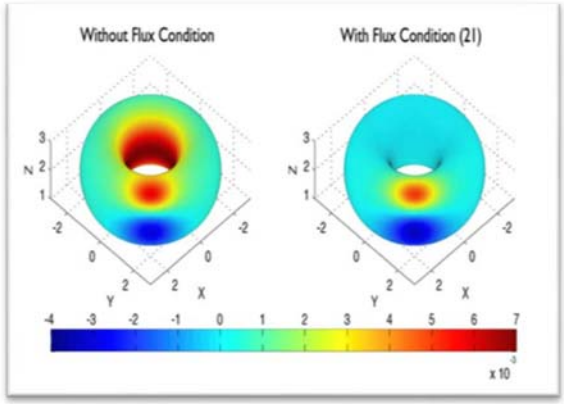
NSSEFF Awardee: Leslie Greengard **Year of Award:** 2010

Project Name: Novel Methods for Electromagnetic Simulation and Design

Dr. Leslie Greengard, a professor in the Courant Institute of Mathematical Sciences at New York University, was awarded an NSSEFF fellowship in 2009 to add new functionality to advanced communication systems, especially with regard to electromagnetic interference. These systems have reached such an advanced stage of complexity that using design by experimentation is impractical. Thus, to avoid electromagnetic interference because of the interaction between antennas, other electromagnetic sources, and the platform itself, accurate computational approaches are required. The techniques developed in this project are sufficiently robust to cope with a broad range of frequencies and detailed geometric models, and they will have to be sufficiently fast to allow design by simulation.

Achievements: This project has resulted in the development of a powerful class of methods for computational electromagnetics, based on new mathematical representations for the Maxwell equations, high-order discretization of surfaces and unknowns, and new fast solvers. This enables high-fidelity simulations of geometrically complex and electrically large objects—which are critical for wideband antenna design, optical component simulation, radar cross section (RCS) prediction, and a host of other electromagnetic-scattering applications. A fully functional simulation environments for micro-structured materials design, planar antenna design, and RCS analysis is in the works.

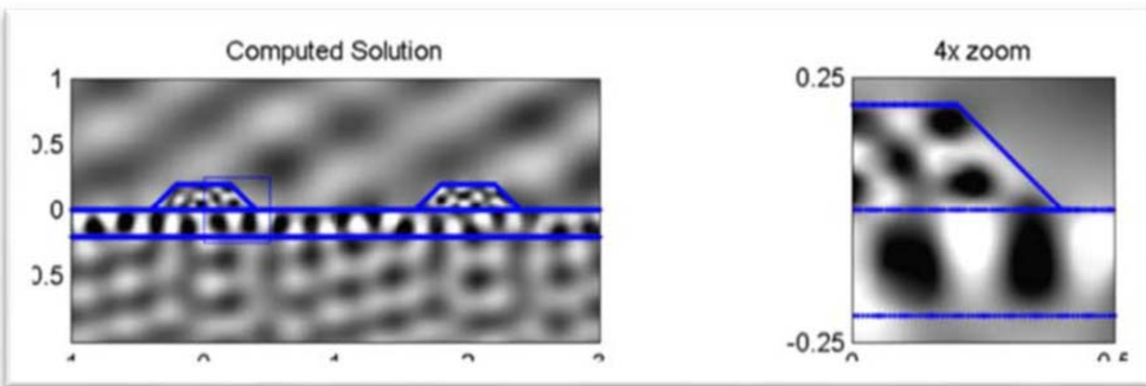
Greengard's team developed a new method to overcome low-frequency breakdown in the magnetic field integral equation that permits accurate reconstruction of the electric field in the near and/or far zones. The team has shown that one can overcome low-frequency breakdown following the solution of the magnetic field integral equation by solving an auxiliary (scalar) integral equation for the charge. This overcomes the ill-conditioning in computing the electric field. Moreover, both the current and charge can be discretized using simple piecewise polynomial basis functions on triangulated surfaces (Epstein et al. 2013). A classical problem in electromagnetics concerns the representation of the electric and magnetic fields scattered from multiply connected conductors in the low-frequency regime, where topology plays a fundamental role. At zero frequency, the standard boundary conditions on the tangential components of the magnetic field do not uniquely determine the vector potential. They have discovered a (gauge-invariant) consistency condition that overcomes this non-uniqueness and resolves a long-standing difficulty in inverting the magnetic field integral equation (Gimbutas and Greengard 2013). Figure 28 shows the induced surface on a torus at low frequency without and with the new consistency condition.



Source: Gimm (2013).

Figure 28. The Induced Surface Current on A Torus at very Low Frequency Using the Classical and New Approach. The solution on the left has lost all digits of accuracy from low-frequency breakdown.

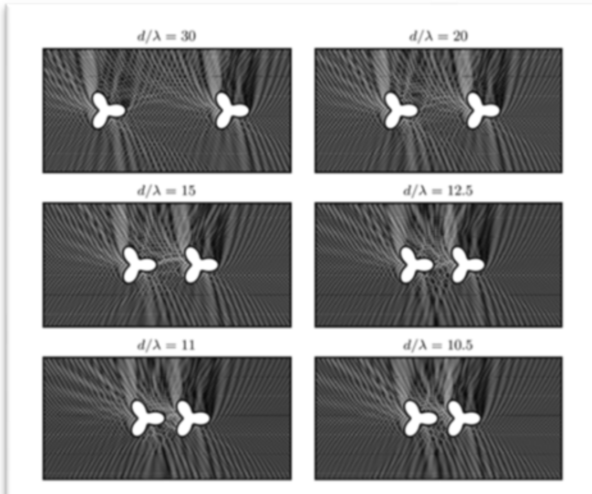
The team has also developed the first robust, well-conditioned integral equation method for the calculation of scattering from periodic and nonperiodic structures involving *triplepoints* (multiple materials meeting at a single point). The combination of a robust and high-order accurate integral representation and a fast direct solver permits the efficient simulation of scattering from fixed structures at multiple angles of incidence (see Figure 29).



Source: Gimm (2013).

Figure 29. The Total Field Scattered by a Periodic Array of Scatters on a Layered Medium. Calculations of this type are common in optics and chip design.

Finally, the team has developed a first generation of fast direct solvers for boundary integral equations in both two and three dimensions, based on combining recursive skeletonization with sparse direct methods (Vico et al. 2013). Figure 30 illustrates the use of the solver in rapidly analyzing the interaction of two objects as they approach each other. The solution time for each scattering geometry was approximately 1 second, using the team's fast direct solver for each scatterer alone as a preconditioner. This is nearly 100 times faster than a standard iterative approach. Thus, as mentioned earlier, these results have important implications for antenna designs, especially with regard to their radar cross section.



Source: Gimm (2013).

Figure 30. The Pressure Field in Response to An Incoming Vertical Plane Wave for Various Scattering Geometries Characterized by Decreasing the Separation Distance Between the Centers of Two Identical Scatterers

Representative Publications

Epstein, C. L., Z. Gimbutas, L. Greengard, A. Klockner, and M. O'Neil. 2013. "A Consistency Condition for the Vector Potential in Multiply-Connected Domains." *IEEE Transactions on Magnetics* 49, no. 3: 1072–1076.

Gimbutas, Z., and L. Greengard. 2013. "Fast Multi-Particle Scattering: A Hybrid Solver for the Maxwell Equations in Microstructured Materials." *Journal of Computational Physics* 232, no. 1: 22–32.

Greengard, L., and J.-Y. Lee. 2012. "Stable and Accurate Integral Equation Methods for Scattering Problems with Multiple Material Interfaces in Two Dimensions." *Journal of Computational Physics* 231, no. 6: 2389–2395.

Ho, K. L., and L. Greengard. 2012."A Fast Direct Solver for Structured Linear Systems by Recursive Skeletonization." *SIAM Journal on Scientific Computing* 34, no. 5: A2507–A2532.

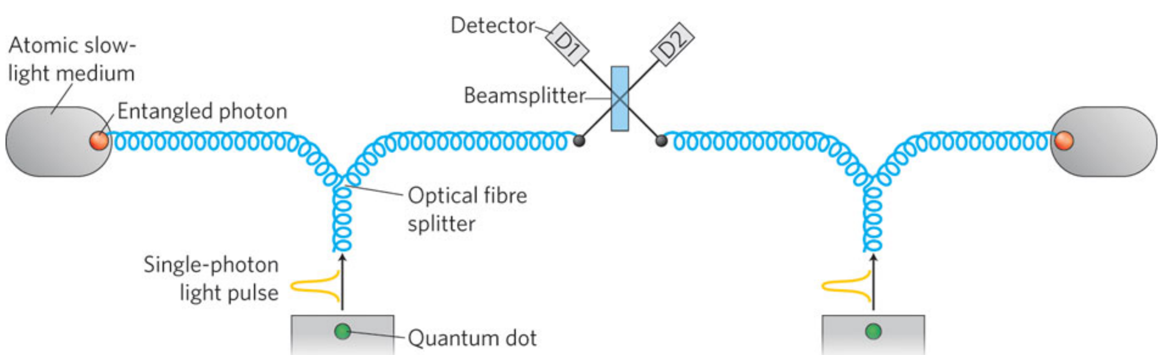
Vico, F., Z. Gimbutas, Z., L. Greengard, and M. Ferrando-Bataller. 2013. "Overcoming Low-Frequency Breakdown of the Magnetic Field Integral Equation." *IEEE Transactions on Antennas and Propagation* 61, no. 3: 1285–1290.

NSSEFF Awardee: Lene Vestergard Hau **Year of Award:** 2010

Project Name: Quantum Control of Light and Matter: from the Macroscopic to the Nanoscale

Dr. Lene Vestergard Hau, the Mallinckrodt Professor of Physics at Harvard University, Cambridge, MA, was awarded an NSSEFF Fellowship in 2010. The goal of the experiments was to use a tiny, supercooled atom cloud called a Bose-Einstein condensate (BEC) to stop the propagation of light pulses and extinguish them. An extinguished light pulse can subsequently be brought back into existence in another BEC in a separate location. The information carried by the light pulse is transferred from the first to the second atom cloud by converting the light pulse into a traveling matter wave, a small atom pulse that is a perfect matter copy of the extinguished light pulse. After the matter wave enters the second BEC, phase locking induced by the presence of that condensate helps restore the original light pulse. While the matter copy is traveling between the two BECs, it can be trapped for extended timescales and reshaped in whatever form required. The induced changes will then be present in the revived light pulse.

Achievements: This research has developed methods that could drive important advances for applications in coherent optical and quantum information processing. For example, the transmission of quantum information can be achieved using similar techniques, but by trapping the light in the quantum state of a quantum dot (see Figure 31). These experiments have given Hau and her students much greater control over quantum information than has been achieved before.



Source: Hau (2011).

Figure 31. A Single Photon is Emitted from Each of the Two Quantum Dots (green) and then Coupled into An Optical Fiber Splitter. Two of the outputs from the fiber splitters are combined at a beam-splitter. When one of the detectors (D1 or D2) clicks and destroys a photon, we do not know at which node (red) the other photon will arrive. The optical modes at these nodes therefore become entangled. Both modes can be coupled to a slow-light medium that introduces a delay. By controlling the delay, the photon in this segment can be synchronized with those in other, similar segments—a technique that allows entanglement to be extended over many segment lengths.

Very large optical nonlinearities can be induced by injecting several light pulses and converting them to matter. By bringing the matter copies into contact, nonlinear effects can be achieved that are many orders of magnitude larger than the nonlinearities that can be achieved with photons alone. They have also built a completely new setup for studies of the interactions between Bose-

Einstein condensates and nanoscale structures, with the aim of creating novel states of cold atomic matter. These experiments have applications for the development of sensitive atom detectors, including chip-integrated devices for atom interferometry, which is important for precise navigation. As a part of this project, new instrumentation and techniques have been developed for fabrication of novel nanoscale structures.

Hau's team also pursued completely new research directions focused on light harvesting with hybrid biosynthetic systems for direct conversion of sunlight to electricity and hydrogen for energy storage. The research combines biological systems with synthetic nanoscale devices and is based on their current studies and experience with light-matter interactions and nanoscale structures.

Representative Publications

Hau, L. V. 2011. "Quantum Optics: Slowing Single Photons." *Nature Photonics* 5: 197–198.

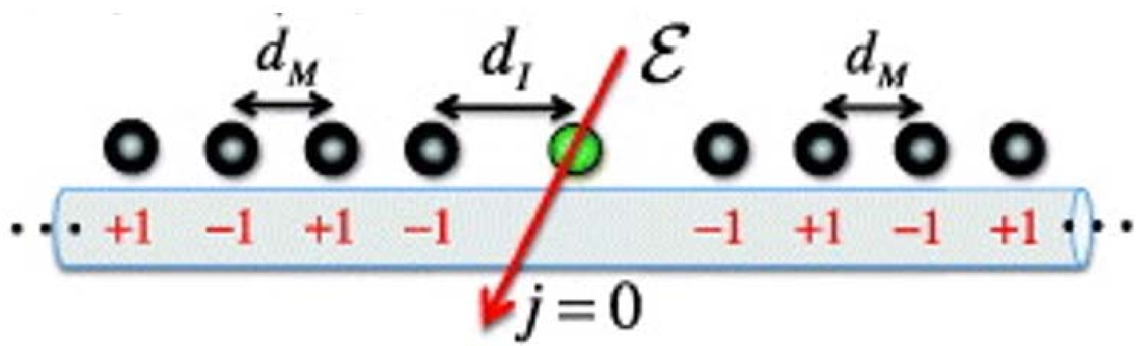
Hau, L. V. 2016. "Manipulating Light." Unit 7 of the Annenberg Foundation's *Physics for the 21st Century*. St. Louis, MO: Annenberg Learner.

NSSEFF Awardee: H. Jeff Kimble **Year of Award:** 2010

Project Name: Quantum networks with Single Atoms, Photons and Phonons

Dr. H. Jeff Kimble, the William L. Valentine Professor and Professor of Physics at the California Institute of Technology, was awarded an NSSEFF Fellowship in 2010 to harness fundamental interactions between light and matter to achieve new capabilities for the processing, storage, and distribution of quantum information. The unifying theme of this research is the realization of the ability to transfer the quantum states of one physical system to states of another system in a reversible fashion. Such capabilities provide the foundation for the implementation of quantum networks for quantum computation, communication, and metrology, as well as for the exploration of exotic quantum phases of matter.

Achievements: This project has had several recent key successes, including several that constitute a revolution in atom-light interaction—specifically, utilizing state-of-the-art theory and nanofabrication processes to produce a new paradigm for the strong interactions of single atoms and photons. An example of these successes is the implementation of a novel technique for enhancing the interaction between light and matter. The technique involves trapping cold atoms near tapered nanofibers, which enables strong coherent coupling between a single atom and a photon. The approach uses collective effects to allow a lattice of atoms to form along the fiber, creating a high-finesse cavity. A specially designed "target" atom within the cavity formed by the "mirror" atoms can experience strongly enhanced interactions with single photons within the fiber (see Figure 32).



Source: Gimm (2013).

Figure 32. An Array of Atoms Trapped by Optical Forces Near the Surface of A Nano-scopic Optical Fiber. Two sets of atoms (the black spheres separated by d_M from each other) become highly reflecting mirrors for light propagating in the fiber. A target atom green sphere is separated by d_I from each of the mirrors. This array can provide a new paradigm for light-matter interactions where the mirrors can form a sort of quantum memory. This is a promising building block for scalable quantum information.

In this way, "strong coupling" can be reached in which quantum-state information can be reversibly exchanged between the "target" atom and a coherent state of the "mirror atoms". This result can provide the basis for a scalable quantum information network using such an “atom-nanofiber” system.

Representative Publications

Chang, D. E., J. I. Cirac, and H. J. Kimble. 2013. “Self-Organization of Atoms along a Nanophotonic Waveguide.” *Physical Review Letters* 110, no. 11: 113606.

Chang, D. E., L. Jiang, A. V. Gorshkov, and H. J. Kimble. 2012. “Cavity QED with Atomic Mirrors.” *New Journal of Physics* 14: 063003.

Goban, A., K. S Choi, D. J. Alton, D. Ding, C. Lacroûte, C., M. Pototschnig, T. Thiele, N. P. Stern, and H. J. Kimble. 2012. “Demonstration of a State-Insensitive, Compensated Nanofiber Trap.” *Physical Review Letters* 109, no. 3: 033603(5).

Hung, C.-L., S. M. Meenehan, D. E. Chang, O. Painter, and H. J. Kimble. 2013. “Trapped Atoms in One-Dimensional Photonic Crystals.” *New Journal of Physics* 15: 083026.

Ni, K.-K., R. Norte, D. J. Wilson, J. D. Hood, D. E. Chang, O. Painter, H. J. Kimble. 2012. “Enhancement of Mechanical *Q* Factors by Optical Trapping.” *Physical Review Letters* 108, no. 21: 214302.

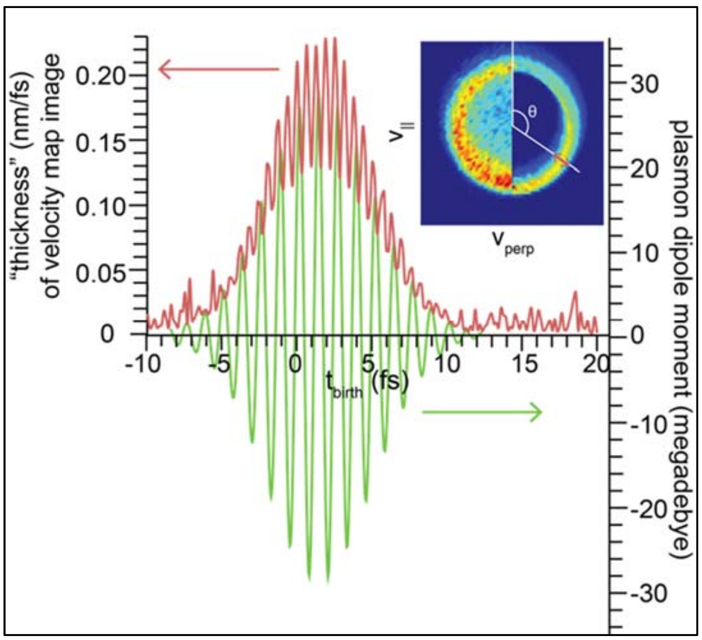
NSSEFF Awardee: Stephen Leone **Year of Award:** 2010

Project Name: Attosecond Electron Processes in Materials: Excitons, Plasmons and Charge Dynamics

Dr. Stephen Leone, the John R. Thomas Endowed Chair in Physical Chemistry and Professor of Chemistry and Physics at the University of California, Berkeley, was awarded an NSSEFF Fellowship in 2010. This award was focused on studying condensed phase electron dynamics on the attosecond (10^{-18} seconds) timescale, the native timescale on which electron dynamics evolve (e.g., motion, coherence, and dephasing). Electronic phenomena such as band gap renormalization in semiconductors, multi-exciton generation in quantum dots, and surface plasmon dephasing in metal nanoparticles were observed in real time as they evolved.

Achievements: Leone achieved the project's goal using state-of-the-art infrared laser pulses lasting only a few optical cycles to generate isolated 100-attosecond bursts of extreme ultraviolet (XUV) light. After initiating an electronic excitation in a solid sample, the attosecond XUV pulses were used to probe the evolution of the excitation after a variable time delay, producing an attosecond-resolved "movie" of the ensuing electron dynamics. Two experimental probe techniques were implemented for this purpose: measurement of the change in the XUV absorption or reflectivity of the sample as a function of pump-probe delay time and measurement of the change in velocity distribution of photoelectrons emitted by the attosecond XUV pulse. Both techniques provided unprecedented insight into processes that govern electron motion in the earliest stages of excitation.

Two instruments for attosecond-resolved electron dynamics experiments have been constructed using this award, with additional support from the W. M. Keck Foundation. Both apparatuses are equipped with 750 nm chirped-pulse amplifiers that produce 25 fs pulses at 1 kHz, with a pulse energy of approximately 1.8 mJ. XUV light is generated by tightly focusing these pulses into a gas cell filled with either neon or argon to produce high harmonics. The spectral bandwidth covered by the resulting XUV pulses can support 100 attosecond pulses. For XUV transient absorption experiments, electron dynamics in solid-state samples are probed by monitoring the change in the transmitted or reflected XUV spectrum at a variable delay time after irradiation of the sample by a 5 fs, 750 nm driving pulse. In velocity map imaging (VMI) experiments, photoelectrons are produced from metallic samples using an XUV pulse at a controlled delay time after initiating a plasmon with the driving pulse, and the velocity distributions of the photoelectrons as a result of their interaction with the plasmon's electric field are imaged. Optics for doubling the 750 nm pulses and temporal compression are being installed to expand the range of accessible pump pulse energies. Using these tools Leone's group has performed experiments that have pushed the frontiers of both attosecond science and solid state physics, incorporating new technologies and theory as part of a comprehensive program. A number of simulations and related experiments were undertaken to augment the instrumental design and data analysis. Many experiments involved the interaction of XUV light with matter irradiated by intense infrared pulses. Experiments and computations performed illustrate that extremely intense infrared light can alter the way that gas-phase atoms transmit XUV light, creating a controllable "switch" for the XUV light that is "on" for times on the order of a femtosecond. We have also shown that intense infrared light pulses can be used to shape attosecond XUV pulses when they are transmitted through a material. In addition, the motion of electrons in atoms and ions excited by light can be tracked experimentally using attosecond XUV pulses. The energy levels in atoms irradiated with intense infrared light can be strongly split due to coupling with the field, and the group has shown that the observed splitting can only be rationalized using a novel new theory. The theoretical and experimental results have provided sophisticated machinery necessary for XUV transient absorption studies. Simulations of photoelectron experiments (see Figure 33) show how velocity map imaging and electron time-of-flight spectrometry can be used to map the temporal and spatial properties of plasmon buildup and decay in metallic nanostructures. The interaction of photoelectrons emitted from silver "nanopillar" samples upon irradiation with intense, few-femtosecond infrared pulses has been studied both experimentally and theoretically.



Source: Gimm (2013).

Figure 33. Simulated Velocity Map Imaging-based Reconstruction of the Dynamical Plasmon Dipole Moment of 80 nm Silver Nanospheres Excited by a Resonant 5 fs, 376 nm Laser Pulse

These results have led to the construction of the world's first solid-state VMI device, which has produced the first attosecond-resolved experimental results. Samples of gold nanodiscs and nanorods resonant at 750 nm have been fabricated in collaboration with the Molecular Foundry at Lawrence Berkeley National Laboratory and their dynamics have been tested on this new instrument.

Representative Publications

Chen, S., M. J. Bell, A. R. Beck, H. Mashiko, M. Wu, A. N. Pfeiffer, M. B. Gaarde, D. M. Neumark, S. R. Leone, and K. J. Schafer. 2012. "Light-Induced States in Attosecond Transient Absorption Spectra of Laser-Dressed Helium." *Physical Review A* 86: 063408.

Leone, S. R., C. W. McCurdy, J. Burgdörfer, L. S. Cederbaum, Z. Chang, N. Dudovich, J. Feist, C. H. Greene, M. Ivanov, R. Kienberger, et al. 2014. "What Will It Take to Observe Processes in 'Real Time'?" *Nature Photon*ics 8, no. 3: 162–166.

Lin, M.-F., A. N. Pfeiffer, D. M. Neumark, S. R. Leone, and O. Gessner. 2012. "Strong-Field Induced XUV Transmission and Multiplet Splitting in $4d^{-1}6p$ Core-Excited Xe Studied by Femtosecond XUV Transient Absorption Spectroscopy." *Journal of Chemical Physics* 137, no. 24: 244305.

Nagel, P. M., J. S. Robinson, B. Harteneck, T. Pfeifer, M. J. Abel, J. S. Prell, D. M. Neumark, R. A. Kaindl, and S. R. Leone. 2013. "Surface Plasmon Assisted Electron Acceleration in Photoemission from Gold Nanopillars." *Chemical Physics* 414: 106–111.

Pfeiffer, A. N., and S. R. Leone. 2012. "Transmission of an Isolated Attosecond Pulse in a Strong-Field Dressed Atom." *Physical Review A* 85: 053422.

NSSEFF Awardee: Todd J. Martinez **Year of Award:** 2010

Project Name: Computational and Theoretical Design of Photo- and Mechano-Responsive Molecular Devices

Dr. Todd Martinez, the D. M. Ehrsam and E. C. Franklin Professor in the Department of Chemistry at Stanford University, was awarded an NSSEFF Fellowship in 2010. This project focused on what some considered a "holy grail" in theoretical chemistry, namely, the ability to design molecular systems with desired functions from first principles. One of the major obstacles in this quest has been the need for methods that are both accurate and computationally efficient, so that a large portion of chemical space can be sampled and explored. This project was aimed at developing new electronic structure and first-principle molecular-dynamics methods that can overcome this obstacle, and applying these methods to design functions into photo- and mechano-activated molecular devices, that is, large molecular structures such as biological macromolecules, polymers, and supramolecular systems.

Achievements: The project developed new tools for chemical simulation, exploiting novel computational architectures such as graphical processing units, as well as new algorithms to reduce computational scaling inspired by advances in machine learning. These new tools are being used to introduce novel approaches such as interactive *ab initio* molecular dynamics, where a human user can guide the simulation to discover new design principles, and "discovery-mode" simulations, where stable structures can be sampled and automatically cataloged along with chemical reactions connecting these stable structures. Finally, these new tools are being applied to excited states in proteins and biomolecules, as well as mechanically induced reactivity in polymeric systems.

Martinez's team developed a graphical processing unit (GPU) based electronic structure theory code (TERACHEM) that made calculations both faster and more accurately than previous systems (Luehr, Ufimtsev, and Martínez 2011). The fast, single-precision calculation capability of the GPU has been exploited with a new "dynamical precision" algorithm that uses single precision for small Coulomb repulsion integrals and double precision for the large integrals. The threshold separating small and large integrals is dynamically adjusted to ensure that the accuracy of the calculation at any given stage is commensurate with the distance from the ultimate solution. Because the solution is determined progressively—that is, the algorithm focuses on the difference between the improved solution and the previous iteration in the electronic structure calculation—this dynamical precision algorithm can achieve double-precision accuracy without *ever* calculating all the Coulomb repulsion integrals in double precision. This algorithm enables calculations to be carried out two to four times faster than the conventional double-precision algorithm, without loss of accuracy. The insight here is far-reaching and applies not only to numerical precision of the computational unit but also to approximations such as the neglect of small exchange matrix elements. Martinez's team is using this idea in a broader context, considering sequences of approximate Hamiltonians that approach the desired Hamiltonian at convergence. As in the dynamical precision case, this has led to acceleration of calculation time without altering the accuracy of the final result.

This team also incorporated the ability to describe electronic excited states in TERACHEM using time-dependent density functional theory. The team carried out the *first* calculations of excited states in a protein, with explicit quantum mechanical treatment of all the $O(10^4)$ electrons in the molecule. The team has used this to calculate absorption spectra of photoactive yellow protein (requiring thousands of calculations, each of which would have been impossible previously). These calculations demonstrate that the convergence of hybrid quantum mechanical/molecular mechanical (QM/MM) methods is quite slow and requires QM treatment of 500 or more atoms in the region surrounding the chromophore. Fortunately, such calculations are now routinely possible due to the team's developments in the algorithms and implementation on GPUs (Isborn et al. 2012).

TERACHEM was used to carry out the first *ab initio* molecular dynamics calculation of a solvated protein molecule and further explored possible failures in the empirical force field descriptions that are dominantly used. The team found that there are significant charge-transfer effects involving protein and solvent that cannot be modeled with an empirical force field. This result implies that charge-transfer effects involving the surrounding solvent may be important in a variety of molecular systems, ranging from biomolecules to polymers (Ufimtsev, Luehr, and Martínez 2011). The Martinez team carried out a validation of *ab initio* methods for macromolecular structures, comparing to results from empirical force fields and experimental crystal structures. The team clearly showed that empirical-force-field results are significantly less trustworthy when biological macromolecules are disordered, while the *ab initio* results remain accurate for both ordered and disordered structures. The deficiency of empirical-force-field-derived structures is expected, since these force fields are parameterized to reproduce well-ordered structures (e.g., alpha-helix and beta-sheet structures in proteins). However, the uniform accuracy of *ab initio* methods could not be securely predicted beforehand. Indeed, some of the density functionals commonly considered as the best for molecular structures and chemical reaction energetics (e.g., B3LYP) become questionable for large molecules (with 200+ atoms). Thus, one of the outcomes of this work was the recognition that range-separated functionals (which remove self-interaction errors exactly for distant electrons) may be required for DFT calculations on large molecules (Kulik, Luehr, Ufimtsev, and Martínez 2012).

This team has also exploited the efficiency of TERACHEM to implement an interactive ab initio molecular dynamics method. A haptic input device allowing the user to control the three-dimensional position of a pointer with full force feedback is combined with TERACHEM, three-dimensional visualization, and the VMD molecular graphics program (Luehr, Jin, and Martínez 2015). *Ab initio* molecular dynamics can be visualized interactively (approximately 1 femtosecond of simulation time every second of real time), and the user can select atoms and pull on them. Strong bonds are harder to break (force feedback form the haptic device is stronger), and the user can feel this. The interface has been improved to make it easier to interact with the molecular simulation. This has turned out to be a useful tool to probe mechanical response of chemical units embedded in mechanosensitive polymers, for probing intermolecular interactions, and for providing human input to guide simulations (e.g., in the context of molecular design). This methodology is illustrated in Figure 34.

Source: Luehr, Jin, and Martínez 2015.

Figure 34. Interactive *Ab Initio* Molecular Dynamics with Haptic Force Feedback

Finally, the team has used machine-learning techniques to develop a new approach to electronic structure theory that reduces the computational scaling with respect to molecular size by *two* orders of magnitude. This translates to an efficiency gain of 250,000 for a molecule with 500 atoms. The idea is based on tensor decomposition of the two-electron repulsion integrals and wave-function coefficients. Fourth-order tensors are represented as a product of five second-order tensors. This "tensor hypercontraction" method has been applied to perturbation theory, configuration interaction, and coupled cluster methods. The team showed that the method reproduces energies obtained from conventional methods to better than chemical accuracy (1 kcal/mol). The team has implemented these methods on GPUs and, in parallel, has made wave-function-based methods for electronic excited states viable for molecules with $O(10^3)$ atoms.

The NSSEFF award allowed Martinez to move into new directions of research not otherwise possible. The fellowship supported "nontraditional" academic staff like programmers, who were critical to the team's success, but would not have been possible with smaller grants. Subsequent research with ONR, ARO, and AFOSR built on the foundation established through the fellowship. This new paradigm developed allowed his team to solve problems by discovery rather than by hypothesis—this was enabled by the use of computer-based nano-reactors. This work allowed for watching chemical dynamics evolve on the computer screen.

Representative Publications:

Hohenstein, E. G., R. M. Parrish, and T. J. Martínez. 2012. "Tensor Hypercontraction Density Fitting. I. Quartic Scaling Second- and Third-Order Møller-Plesset Perturbation Theory." *The Journal of Chemical Physics* 137 (4): 044103.

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Luehr, N., I. S. Ufimtsev, and T. J. Martínez. 2011. "Dynamic Precision for Electron Repulsion Integral Evaluation on Graphical Processing Units (GPUs)." *Journal of Chemical Theory and Computation* 7 (4), 949–954.

Ufimtsev, I. S., N. Luehr, and T. J. Martínez. 2011. "Charge Transfer and Polarization in Solvated Proteins from *Ab Initio* Molecular Dynamics." *The Journal of Physical Chemistry Letters* 2 (14), 1789–1793.

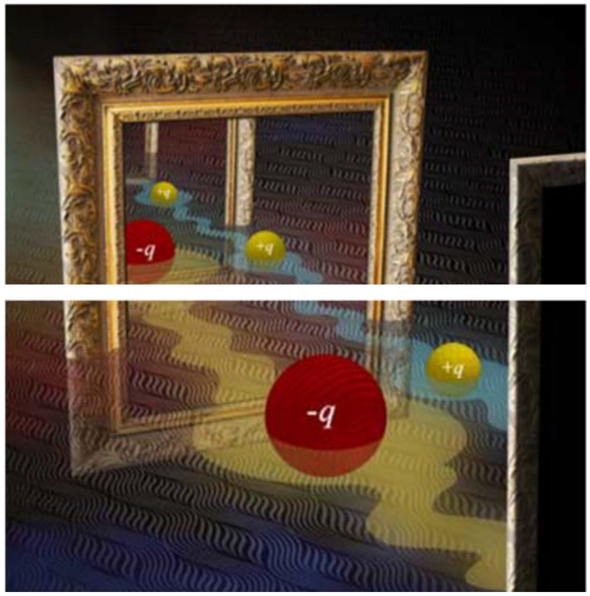
NSSEFF Awardee: Monica Olvera de la Cruz **Year of Award:** 2010

Project Name: Paradigms for Emergence of Shape and Function in Biomolecular Electrolytes for the Design of Biomimetic Materials

Dr. Monica Olvera de la Cruz, the Lawyer Taylor Professor of Materials Science and Engineering at Northwestern University, was awarded an NSSEFF Fellowship in 2010. This award was focused on uncovering the principles underlying the cellular programming responsible for compartmentalization, communication, and replication, as well as subsequently employing these principles to generate assemblies that function as autonomous organisms.

Achievements: The NSSEFF award allowed de la Cruz to change how she conducted research, which enabled her to frame a new form of electrostatics based on a LaGrangian form that allowed her to expand the formalism to develop the molecular dynamics simulations of charged living systems. Living matter is highly inhomogeneous at the nano-scale, both in composition and charge. A big challenge has been to determine how these inhomogeneities generate functions. In this context, the dominant role played by electrostatics during pattern formation is evident, given that nucleic acids and many proteins are charged or possess units with tunable degrees of charge. As a result, the association of biomolecules into functional units has demonstrated strong dependence on local ionic concentrations. Thus, using ionic gradients as one means to control the assembly and disassembly of biological entities is critically important to generating biomimetic functions. De la Cruz and her team developed models, based on information collected in vivo and in situ, to better understand the physical properties and functions of biomolecular assemblies in different ionic conditions for designing biomimetic materials with new capabilities.

This project studied fluids of charged particles that acted as the supporting medium for chemical reactions and physical, dynamical, and biological processes. Micro- and nano-scopic polarizable objects deform the local structure in an electrolytic background. Likewise, the forces between the objects are regulated by the cohesive properties of the background (see Figure 35). The team studied the range and strength of these forces and the microscopic origin from which they emerge (Funkhouser et al. 2013), providing an intuitively appealing overview to aid and enhance predictability and control in experiments. The authors described several distinct ion-induced forces in aqueous solutions of monovalent ions at salt concentrations ranging from 0.01 to 1 M that are expected to compete for dominance with the well-known screened Coulomb forces. The concept of soft structure was introduced to connect the induced forces to the local microscopic structure in the ionic fluid and visualize the deformation of the local environment around the ions near several types of boundaries that are neutral, absorbing, charged, polarizable, or a combination of these properties. Until recently, it was computationally costly to simulate the effects of charges on inhomogeneous dielectric media and vice versa, since it required solving the Poisson equation at each simulation step.

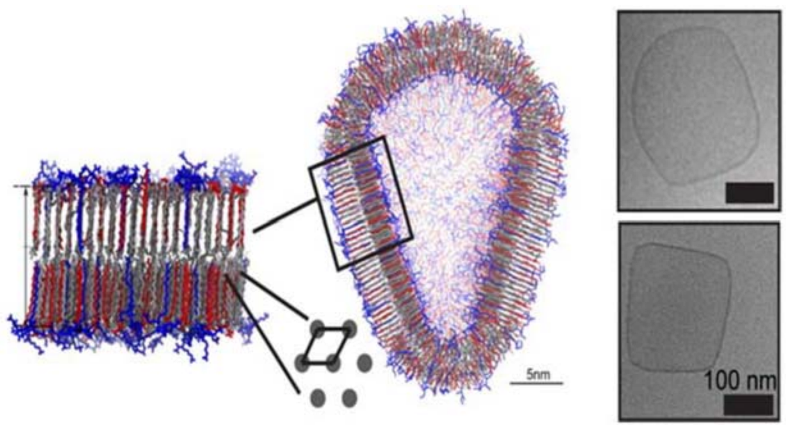


Source: Artistic impression by D. Spjut.

Figure 35. Charged Particles in A Liquid are Enveloped by a Cloud of Opposite Charge that Deforms Near Boundaries, and Creates a Force Qway from the Boundary. Electrostatically, boundaries act as mirrors, causing additional attractions or repulsions. Theory reveals how ions influence forces between boundaries in an intricate way, and vice versa, with important implications for biological systems.

In a related study, the de la Cruz team developed a judiciously designed variational formulation, eliminating the need to solve the Poisson equation explicitly. This work led to tremendous speedups in simulations of charged systems. Much of the structural stability of the cell's nucleus comes from meshwork of intermediate filament proteins known as lamins, which form the inner layer of the nuclear envelope called the nuclear lamina. These lamin meshwork additionally play a role in gene expression. Abnormalities in nuclear shape are associated with a variety of pathologies, including some forms of cancer and Hutchinson–Gilford progeria syndrome, and often include protruding structures termed nuclear blebs. These nuclear blebs are related to pathological gene expression. However, little is known about how and why blebs form. De la Cruz's team developed a minimal continuum elastic model of a lamin meshwork that was used to investigate which aspects of the meshwork could be responsible for bleb formation. The model produces structures with comparable morphologies and distributions of lamin types as in real pathological nuclei (Leung et al. 2013). Thus, preventing this lamin segregation could be a route to prevent bleb formation, which could be used as a potential therapy for the pathologies associated with nuclear blebs.

A considerable part of the NSSEFF work was aimed at elucidating the structure and function relationship in membranes. A large variety of amphiphillic molecules with charged groups self-assemble into closed structures such as viral capsids, halophilic organisms, and bacterial microcompartments. The team formulated a generalized elastic model for inhomogeneous shells and demonstrated that coassembled shells with two elastic components buckle into irregular and regular polyhedra besides icosahedra, such as dodecahedra, octahedra, tetrahedra, and hosohedra shells. The mechanism with which this occurs explains many observations, predicts a new family of polyhedral shells, and provides the principles for designing micro-containers with specific shapes and symmetries for numerous applications in materials and life sciences (Li et al. 2012). For instance, designing polyhedral shells with specific structures can lead to efficient nano-reactors that will perform specific catalytic functions. In a combined effort with other Northwestern collaborators, the team modeled and assembled shells composed of oppositely charged lipids, and were able to regulate the shape of the resulting nanocontainers via pH changes, as evidenced by transmission electron microscopy (TEM; see Figure 36) and X-ray scattering (Vernizzi, Sknepnek, and de la Cruz. 2011). Vesicles or nano-containers with crystalline properties show great promise in nanomaterial fabrication due to their excellent mechanical stability in high-salt-concentration environments.



Source: Gimm (2013).

Figure 36. Atomistic Simulations, and TEM Images of Faceted and Irregular Polyhedral with Hexagonal Crystalline Symmetry, Stable in Closed Shaped and High Salt Concentration

The team also studied, by atomistic simulations, the effects of counterion valency on anionic membranes. This work showed that the inter-tail van der Waals interaction has a dominant role in the electrostatic-driven transition from disordered liquid crystalline phase to the ordered gel phase. Using monovalent counterions, such phase transitions occur at lower temperatures than in scenarios where multivalent counterions are used. The team also studied the effects of curvature in multi-component liquid membranes with three components using molecular dynamics simulations to find low-energy structures. The different chemical and physical properties of the components, whose shapes and in-membrane arrangement are coupled through phase-specific bending energies and line tensions, results in a variety of shapes and component patterns. Moreover, the team studied shapes of pored membranes and showed that the mean curvature leads to budding-like behavior, while the Gaussian curvature flattens membranes near the pore area. The de la Cruz team's work explains shapes of pored membranes that are observed in experiments.

Motivated by the remarkable stability against degradation by nucleases of functionalized spherical nuclei acids-gold (SNA-Au) nanoparticles in blood, the team modeled the ion cloud around them by means of classical density functional theory and by computer simulations. For small particles with high density of oligonucleotides, the team found that the local salt concentration is enhanced with a pronounced localization of divalent ions near the particle surface. This strong cloud of sodium and calcium ions stabilizes the particle complex in blood, which may prevent enzymes from accessing the DNA and digesting it. The team also developed coarse-grained schemes to understand and optimize programmable assembly (Zwanikken and de la Cruz. 2013) of grafted nuclei acid-gold nanoparticles. In particular, the team's molecular dynamics simulations have identified key elements, such as optimal strength of DNA linkers and percentage of DNA hybridizations, to successfully assemble nanoparticles into a large variety of superlattices. The molecular dynamics simulations have also elucidated the role that nanostructure coordination plays in the ordering of superlattice assemblies. Detailed phase diagrams that were constructed to closely match the experimental observations showed that highly dynamic hybridization processes between the semi-flexible grafted chains enable crystallization of the functionalized nanoparticles. A model that efficiently captures the competing electrostatic and DNA hybridization interactions in the assembly process was developed to determine the dynamics of the coarsening process that leads to various faceted crystals of functionalized nanoparticles.

Representative Publications:

Funkhouser, C. M., R. Sknepnek, T. Shimi, A. E. Goldman, R. D. Goldman, M. Olvera de la Cruz. 2013. "Mechanical Model of Blebbing in Nuclear Lamin Meshworks." *Proceedings of the National Academy of Sciences* 110, no. 9: 3248–3253.

Leung, C-Y., L. C. Palmer, B. F Qiao, S. Kewalramani, R. Sknepnek, C. J. Newcomb, M. A. Greenfield, G. Vernizzi, S. I. Stupp, M. J. Bedzyk, and M. Olvera de la Cruz. 2012. "Molecular Crystallization Controlled by pH Regulates Mesoscopic Membrane Morphology." *ACS Nano* 6, no. 12: 10901–10909.

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Vernizzi, G., R. Sknepnek, and M. Olvera de la Cruz. 2011. "Platonic and Archimedean Geometries in Multicomponent Elastic Membranes." *Proceedings of the National Academy of Sciences* 108, no. 11: 4292–4296.

Zwanikken, J. W., and M. Olvera de la Cruz. 2013. "Tunable Soft Structure in Charged Fluids Confined by Dielectric Interfaces." *Proceedings of the National Academy of Sciences* 110, no. 14: 5301–5308.

NSSEFF Awardee: Lenya Ryzhik **Year of Award:** 2010

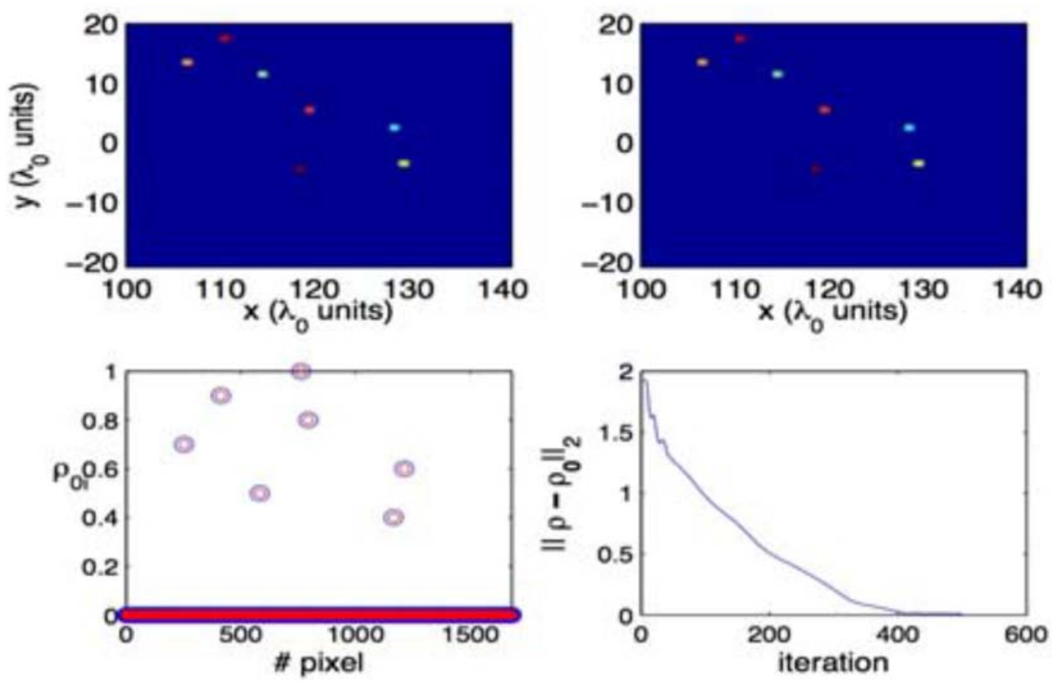
Project Name: Mathematical Modeling in Random Media – From Homogenization to Stochasticity

Dr. Lenya Ryzhik, professor in the Department of Mathematics of Stanford University, was awarded an NSSEFF Fellowship in 2010. The goal of this fellowship was to understand the propagation of uncertainty from a priori unknown coefficients in partial differential equations (PDEs) to solutions of such equations. The underlying equations model a variety of phenomena such as propagation of waves in heterogeneous media (e.g., radars) or heat distribution or electric current in a nonuniform medium. The unifying aspect of these problems is that the physical parameters in the system cannot be perfectly known because of the fluctuations and small-scale heterogeneities. Such phenomena are ubiquitous in nature, and the basic problem that is of both theoretical and practical importance is quantifying the effect of uncertainty at the microscopic scales on the macroscopic phenomena. Such understanding is critical in parameter estimation—where one is interested in recovering the macroscopic properties of a complex medium but not the fine-scale oscillations—as well as in problems where the goal is to use remote measurements to find an object hidden in a medium and obscured by the heterogeneities.

Achievements: The core objective of this research involved the fluctuations in the available measurements beyond the homogenization limit and how the fluctuations depend on the randomness in the coefficients of the PDE. Such fundamental questions turn out to be particularly challenging. Only in some PDE models is there a complete understanding of this problem—with major contributions from this research. Mathematically, the uncertainty in the medium parameters that cannot, and should not, be reconstructed is modeled as *noise*. Both the forward and inverse problems then hinge on two fundamental questions: (1) find measurements that are as immune to effects of *noise* as possible, and (2) understand how *noise* propagates up to the macroscopic scales and affects the large-scale phenomena. The work for this fellowship was done by the L. Ryzhik group at Stanford and the G. Bal group at Columbia University.

A homogenization regime arises when medium properties have short-range correlations, so that the random coefficients rapidly “forget” values at nearby points. In contrast, media with slowly decaying correlations are fractal and have structure on all scales. A major accomplishment of this research is the discovery of the dichotomy between these regimes; that is, solutions of PDEs exhibit drastically different behavior in these two types of media. One important class of PDEs for which this analysis has been carried out is parabolic equations with random potentials. This class includes the parabolic models of radars in turbid environments. For such models, both when the random potential is strong and weak, it was discovered that the propagation of stochasticity strongly depends on the decorrelation properties of the random potential. For potentials with short-range correlations, the team observed that the PDE solution converged to a homogenized solution, as predicted by homogenization theory. Moreover, the random fluctuations in the PDE solution can be asymptotically described by a stochastic PDE with additive noise or random initial data. This completely characterizes the propagation of stochasticity in this case. In contrast, for a potential with long-range correlations, the team has shown that the PDE solution remained stochastic at the macroscopic level, and in the case of weakly random potentials affect the solution in a nontrivial way on a timescale much shorter than that for rapidly decorrelating potentials. The team has also discovered the completely new phenomenon: long-range correlations introduce a continuum of temporal scales on which various observables become nontrivially affected. For instance, the wave amplitude becomes randomized on a timescale much shorter than the phase. This dramatically effects our understanding of which wave functionals should be measured in turbid media. Similar results were obtained for other PDE models, including those used in propagation of waves in complex media. The salient feature of such results is a characterization of the effect of the correlation properties of a random medium on the stochasticity of the PDE solutions.

Imaging in Weakly Heterogeneous Media. The team has developed a new imaging algorithm (i.e., generalized Lagrangian multiplier algorithm, or GeLMA) that employs the idea that typically the objects that one needs to find in a complex medium are sparse (Moscoso et al. 2012). GeLMA is based on an ordinary differential equation formulation of an l1-minimization problem and works extremely well even in the presence of a relatively strong noise. Introduction of the a priori information (sparsity) into the imaging problem dramatically accelerates the rate of convergence in complex media (see Figure 37).



Source: Moscoso et al. 2012.

Figure 37. Top row: Original configuration of the scatterers (left) and the recovered image with GeLMA (right). Bottom row, left: Comparison between the exact solution (large blue circles) and the GeLMA solution (small red circles). Bottom row, right: Convergence rate of the GeLMA algorithm.

The propagation of waves in heterogeneous media is another example of a problem modeled by a PDE involving random and highly oscillatory coefficients. One central component of this research is to understand, and whenever possible rigorously justify, how stochasticity propagates from the coefficients in the PDE to its solution. As described above, measurements are functionals of the solutions to the PDE, and the errors committed in the reconstructions of parameters of interest are directly related to errors in measurements. All limitations in parameter estimations are therefore to a large extent driven by how stochasticity propagates from noise to measurements. The analysis of such models has a long history, both in the mathematical and engineering communities. However, most work there is done in the so-called homogenization regime, where randomness in coefficients affects solutions of PDEs in a highly nontrivial way, but nevertheless solutions are nearly deterministic. This regime is valid when the random fluctuations oscillate on a much smaller scale than the macroscopic size of the domain of interest (in Figure 37, the domain is 200 times larger than the microscopic scale given by the wavelength of the waves). This regime is crucial because it provides a model on how measurements depend on the parameters of interest (e.g., the buried inclusion in the preceding example). Note, however, that it gives no information about the size of the inevitable random fluctuations in measurements that arise as soon as one moves slightly away from the homogenization regime, as always happens in practice.

Representative Publications

Bal, G., and O. Pinaud. 2011. “Imaging Using Transport Models for Wave–Wave Correlations.” *Mathematical Models and Methods in Applied Sciences* 21 (5): 1071–1093.

Bal, G., O. Pinaud, L. Ryzhik, and K. Sølna. 2014. “Precursors for Waves in Random Media.” *Wave Motion* 51 (8): 1237–1253.

Komorowski, T., and L. Ryzhik. 2014. “Long Time Energy Transfer in the Random Schrödinger Equation.” *Communications in Mathematical Physics* 329 (3): 1131–1170.

Moscoso, M., A. Novikov, G. Papanicolaou, and L. Ryzhik. 2012. “A Differential Equations Approach to l_1-Minimization with Applications to Array Imaging.” *Inverse Problems* 28 (10): 105001.

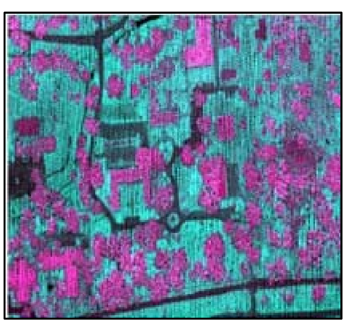
NSSEFF Awardee: Guillermo Sapiro **Year of Award:** 2010

Project Name: Information Acquisition, Analysis and Integration

Dr. Guillermo Sapiro, Edmund T. Pratt, Jr. School Professor of Electrical and Computer Engineering at Duke University, was awarded an NSSEFF Fellowship in 2010 to develop novel theoretical, computational, and practical theories and frameworks to exploit the extraordinarily voluminous video and image data being continually produced by various sources (e.g., YouTube, security videos, sensor imaging). Examples of the types of data whereby improved analysis would be beneficial include geotagged images from around the world, security/surveillance monitoring systems, and medical/neuroscience imagery.

Achievements: The research has developed novel algorithms and representations for multidimensional and multimodal data to facilitate analysis and improve subsequent deeper understanding of the data. The project has worked to build fundamental tools covering numerous areas of science, moving away from more common ad-hoc approaches that have dominated imagery data representation.

With geotagged imagery, Sapiro and colleagues developed a method using LiDAR images that provide elevation readings along with hyperspectral images that provide enhanced imaging capabilities (Castrodad et al. 2012). Images that exceed the visual spectrum allow for the identification of edges based on different properties across the electromagnetic spectrum (e.g., reflectance of visible light or temperature fluctuations from the infrared spectrum). The addition of LiDAR imaging provides the distance of objects from the sensor. Combining these methods allows for greater understanding of the geographical features in the image. For example, the dark green of tree leaves might be similar to dark green grass in the shadow of the tree, but differentiating those two would be possible by examining differences in elevation captured through LiDAR or cooler temperatures in the shade captured through infrared imaging.



(a)

(b)

(c)

Source: Castrodad et al. 2012.

Figure 38. (a) Fusion of Depth-Intensity-Average Map from LiDAR; (b) with a Hyperspectral Image; (c) to Produce an HSI-LiDAR Fused Scene

Sapiro has also worked to develop techniques that can parse the components of video, separating the foreground objects from the background (Newson, Tepper, and Sapiro 2015). The novel technique includes segmenting the video so that local component analysis is possible, which allows the system to account for complex lighting conditions and variability in the background. Then the small spatio-temporal regions are merged to produce a coherent background.

Sapiro's research has also benefited medical imaging capabilities. For example, magnetic resonance imaging (MRI) allows for high-resolution imaging inside a person's body, but has some limitations that are being addressed. One such limitation of neural imaging of the brain has been the ability to identify the pathway of neurons that transmit information across the brain. By manipulating the angle of magnetic fields and adjusting the signal-to-noise ratio of filters for each image, the system can detect fibers crossing at particular angles in a voxel (i.e., a three-dimensional element from a volume image, analogous to a pixel in a two-dimensional image). Then, by comparing results in surrounding voxels, the system can identify the pathway of neuronal fibers. This form of image processing is computing-resource intensive, and the method developed by Sapiro and his collaborators have demonstrated a reduction in sampling by a factor of 4 (Duarte-Carvajalino et al. 2014), which may greatly increase the utility of imagining for medical procedures.

Sapiro's development of methods and algorithms has worked to speed up processing or to gain additional information that had not been realized before. Some of Sapiro's work is now being leveraged by commercial entities like Adobe, and he has continued to conduct research for DoD. The basic research conducted by Sapiro will contribute to the ability to better analyze the wealth of video and still-image data that are constantly being collected and that the military needs to better understand.

Representative Publications

Castrodad, A., T. Khuon, R. Rand, R., G. Sapiro. 2012. "Sparse Modeling for Hyperspectral Imagery with LIDAR Data Fusion for Subpixel Mapping." Paper presented at the 2012 IEEE International Geoscience and Remote Sensing Symposium, Munich, Germany, 22–27 July.

Duarte-Carvajalino, J. M., C. Lenglet, J. Xu, E. Yacoub, K. Ugurbil, S. Moeller, L. Carin, and G. Sapiro. 2014. "Estimation of the CSA-ODF Using Bayesian Compressed Sensing of Multi-Shell HARDI." *Magnetic Resonance in Medicine* 72 (5): 1471–1485.

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Abbreviations

2D	two-dimensional
3D	three-dimensional
AFOSR	Air Force Office of Scientific Research
ASSIST	Advanced Self-Powered Systems of Integrated Sensors and Technology
BEC	Bose-Einstein condensate
CHA	catalyzed hairpin assembly
CMOS	complementary metal oxide semiconductor
CV-N	Cyanovirin-N
DARPA	Defense Advanced Research Projects Agency
DFT	density function theory
DMFT	dynamical mean field theory
DNA	deoxyribonucleic acid
DoD	Department of Defense
EAGER	Early Concept Grants for Exploratory Research
ECG	electrocardiography
EEG	electro-encephalography
EQE	external quantum efficiency
FDTD	finite-difference time-domain
GaAs	gallium arsenide
GPa	gigapascal
GPU	graphical processing unit
HBCUs	Historically Black Colleges and Universities
HHG	high harmonic generation
HIV	human immunodeficiency virus
IDA	Institute for Defense Analyses
InGaAs	indium gallium arsenide
LaMnPO	an antiferromagnetic semiconductor
LED	light-emitting diode
LiDAR	light detection and ranging
LUCI	Laboratory University Collaboration Initiative
MEMS	microelectromechanical systems
Mn	manganese
MnP	manganese peroxidase
MOT	magneto-optic trap
MRI	magnetic resonance imaging
MURI	multidisciplinary university research initiative
nanoES	nano-electronic scaffolds
nano-FET	nanoscale field effect transistor
NP	nanopillars

NSF	National Science Foundation
NSSEFF	National Security Science and Engineering Faculty Fellowship
NWs	nanowires
ONR	Office of Naval Research
OSD	Office of the Secretary of Defense
OSD-DURIP	Office of the Secretary of Defense – Defense University Research Instrumentation Program
OWL	on-wire-lithography
PDEs	partial differential equations
PE	Program Element
PI	principal investigator
PZT	(also known as) lead zirconate titanate
QM/MM	quantum mechanical/molecular mechanical
QRS	refers to individual waves in an ECG
RCS	radar cross section
RF	radio-frequency
Scalar	solving an auxiliary
SEM	scanning electron microscope
SERS	surface enhanced Raman spectroscopy (or scattering)
SHG	second harmonic generated
SNA-Au	spherical nuclei acids-gold
STEM	science, technology, engineering, and mathematics
TEM	transmission electron microscopy (
TERACHEM	electronic structure theory code
Tx	transmit antenna
VBFF	Vannevar Bush Faculty Fellowship
VCSEL	vertical cavity surface emitting laser
VMD	Visual Molecular Dynamics (software program)
VMI	velocity map imaging
XUV	extreme ultraviolet

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14. ABSTRACT

The Department of Defense established the National Security Science and Engineering Faculty Fellowships (NSSEFF) program in 2008 to support university faculty and scientists to conduct potentially high pay-off basic research. In 2016, the name of the program was formally changed to the Vannevar Bush Faculty Fellowship (VBFF) to commemorate Dr. Vannevar Bush's role in directing DoD research and pioneering research for the Government. The research funded through NSSEFF led to the development of several innovative discoveries. The report includes a set of recommendations for the program.

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