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University of Utah	University of Utah 75 South 2000 East Salt Lake City, UT. 841128930
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TITLE OF PROPOSED PROJECT **University of Utah Materials Research Science and Engineering Center**

REQUESTED AMOUNT	PROPOSED DURATION (1-60 MONTHS)	REQUESTED STARTING DATE	SHOW RELATED PRELIMINARY PROPOSAL NO. IF APPLICABLE
$ 2	60 months	09/01/17	

THIS PROPOSAL INCLUDES ANY OF THE ITEMS LISTED BELOW

☐ BEGINNING INVESTIGATOR (GPG I.G.2)
☐ DISCLOSURE OF LOBBYING ACTIVITIES (GPG II.C.1.e)
☐ PROPRIETARY & PRIVILEGED INFORMATION (GPG I.D, II.C.1.d)
☐ HISTORIC PLACES (GPG II.C.2.j)
☐ VERTEBRATE ANIMALS (GPG II.D.6) IACUC App. Date ________
PHS Animal Welfare Assurance Number ________
☒ FUNDING MECHANISM **Research - other than RAPID or EAGER**

☐ HUMAN SUBJECTS (GPG II.D.7) Human Subjects Assurance Number ________
Exemption Subsection ________ or IRB App. Date ________
☐ INTERNATIONAL ACTIVITIES: COUNTRY/COUNTRIES INVOLVED (GPG II.C.2.j)
☒ COLLABORATIVE STATUS
Not a collaborative proposal

PI/PD DEPARTMENT	PI/PD POSTAL ADDRESS
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CERTIFICATION PAGE

Certification for Authorized Organizational Representative (or Equivalent) or Individual Applicant

By electronically signing and submitting this proposal, the Authorized Organizational Representative (AOR) or Individual Applicant is: (1) certifying that statements made herein are true and complete to the best of his/her knowledge; and (2) agreeing to accept the obligation to comply with NSF award terms and conditions if an award is made as a result of this application. Further, the applicant is hereby providing certifications regarding conflict of interest (when applicable), drug-free workplace, debarment and suspension, lobbying activities (see below), nondiscrimination, flood hazard insurance (when applicable), responsible conduct of research, organizational support, Federal tax obligations, unpaid Federal tax liability, and criminal convictions as set forth in the NSF Proposal & Award Policies & Procedures Guide,Part I: the Grant Proposal Guide (GPG). Willful provision of false information in this application and its supporting documents or in reports required under an ensuing award is a criminal offense (U.S. Code, Title 18, Section 1001).

Certification Regarding Conflict of Interest

The AOR is required to complete certifications stating that the organization has implemented and is enforcing a written policy on conflicts of interest (COI), consistent with the provisions of AAG Chapter IV.A.; that, to the best of his/her knowledge, all financial disclosures required by the conflict of interest policy were made; and that conflicts of interest, if any, were, or prior to the organization's expenditure of any funds under the award, will be, satisfactorily managed, reduced or eliminated in accordance with the organization's conflict of interest policy. Conflicts that cannot be satisfactorily managed, reduced or eliminated and research that proceeds without the imposition of conditions or restrictions when a conflict of interest exists, must be disclosed to NSF via use of the Notifications and Requests Module in FastLane.

Drug Free Work Place Certification

By electronically signing the Certification Pages, the Authorized Organizational Representative (or equivalent), is providing the Drug Free Work Place Certification contained in Exhibit II-3 of the Grant Proposal Guide.

Debarment and Suspension Certification

(If answer "yes", please provide explanation.)

Is the organization or its principals presently debarred, suspended, proposed for debarment, declared ineligible, or voluntarily excluded from covered transactions by any Federal department or agency? Yes ☐ No ☒

By electronically signing the Certification Pages, the Authorized Organizational Representative (or equivalent) or Individual Applicant is providing the Debarment and Suspension Certification contained in Exhibit II-4 of the Grant Proposal Guide.

Certification Regarding Lobbying

This certification is required for an award of a Federal contract, grant, or cooperative agreement exceeding $100,000 and for an award of a Federal loan or a commitment providing for the United States to insure or guarantee a loan exceeding $150,000.

Certification for Contracts, Grants, Loans and Cooperative Agreements

The undersigned certifies, to the best of his or her knowledge and belief, that:
(1) No Federal appropriated funds have been paid or will be paid, by or on behalf of the undersigned, to any person for influencing or attempting to influence an officer or employee of any agency, a Member of Congress, an officer or employee of Congress, or an employee of a Member of Congress in connection with the awarding of any Federal contract, the making of any Federal grant, the making of any Federal loan, the entering into of any cooperative agreement, and the extension, continuation, renewal, amendment, or modification of any Federal contract, grant, loan, or cooperative agreement.
(2) If any funds other than Federal appropriated funds have been paid or will be paid to any person for influencing or attempting to influence an officer or employee of any agency, a Member of Congress, an officer or employee of Congress, or an employee of a Member of Congress in connection with this Federal contract, grant, loan, or cooperative agreement, the undersigned shall complete and submit Standard Form-LLL, ''Disclosure of Lobbying Activities,'' in accordance with its instructions.
(3) The undersigned shall require that the language of this certification be included in the award documents for all subawards at all tiers including subcontracts, subgrants, and contracts under grants, loans, and cooperative agreements and that all subrecipients shall certify and disclose accordingly.

This certification is a material representation of fact upon which reliance was placed when this transaction was made or entered into. Submission of this certification is a prerequisite for making or entering into this transaction imposed by section 1352, Title 31, U.S. Code. Any person who fails to file the required certification shall be subject to a civil penalty of not less than $10,000 and not more than $100,000 for each such failure.

Certification Regarding Nondiscrimination

By electronically signing the Certification Pages, the Authorized Organizational Representative (or equivalent) is providing the Certification Regarding Nondiscrimination contained in Exhibit II-6 of the Grant Proposal Guide.

Certification Regarding Flood Hazard Insurance

Two sections of the National Flood Insurance Act of 1968 (42 USC §4012a and §4106) bar Federal agencies from giving financial assistance for acquisition or construction purposes in any area identified by the Federal Emergency Management Agency (FEMA) as having special flood hazards unless the:
(1) community in which that area is located participates in the national flood insurance program; and
(2) building (and any related equipment) is covered by adequate flood insurance.

By electronically signing the Certification Pages, the Authorized Organizational Representative (or equivalent) or Individual Applicant located in FEMA-designated special flood hazard areas is certifying that adequate flood insurance has been or will be obtained in the following situations:
(1) for NSF grants for the construction of a building or facility, regardless of the dollar amount of the grant; and
(2) for other NSF grants when more than $25,000 has been budgeted in the proposal for repair, alteration or improvement (construction) of a building or facility.

Certification Regarding Responsible Conduct of Research (RCR)
(This certification is not applicable to proposals for conferences, symposia, and workshops.)

By electronically signing the Certification Pages, the Authorized Organizational Representative is certifying that, in accordance with the NSF Proposal & Award Policies & Procedures Guide, Part II, Award & Administration Guide (AAG) Chapter IV.B., the institution has a plan in place to provide appropriate training and oversight in the responsible and ethical conduct of research to undergraduates, graduate students and postdoctoral researchers who will be supported by NSF to conduct research.
The AOR shall require that the language of this certification be included in any award documents for all subawards at all tiers.

CERTIFICATION PAGE - CONTINUED

Certification Regarding Organizational Support

By electronically signing the Certification Pages, the Authorized Organizational Representative (or equivalent) is certifying that there is organizational support for the proposal as required by Section 526 of the America COMPETES Reauthorization Act of 2010. This support extends to the portion of the proposal developed to satisfy the Broader Impacts Review Criterion as well as the Intellectual Merit Review Criterion, and any additional review criteria specified in the solicitation. Organizational support will be made available, as described in the proposal, in order to address the broader impacts and intellectual merit activities to be undertaken.

Certification Regarding Federal Tax Obligations

When the proposal exceeds $5,000,000, the Authorized Organizational Representative (or equivalent) is required to complete the following certification regarding Federal tax obligations.
By electronically signing the Certification pages, the Authorized Organizational Representative is certifying that, to the best of their knowledge and belief, the proposing organization:
(1) has filed all Federal tax returns required during the three years preceding this certification;
(2) has not been convicted of a criminal offense under the Internal Revenue Code of 1986; and
(3) has not, more than 90 days prior to this certification, been notified of any unpaid Federal tax assessment for which the liability remains unsatisfied, unless the assessment is the subject of an installment agreement or offer in compromise that has been approved by the Internal Revenue Service and is not in default, or the assessment is the subject of a non-frivolous administrative or judicial proceeding.

Certification Regarding Unpaid Federal Tax Liability

When the proposing organization is a corporation, the Authorized Organizational Representative (or equivalent) is required to complete the following certification regarding Federal Tax Liability:

By electronically signing the Certification Pages, the Authorized Organizational Representative (or equivalent) is certifying that the corporation has no unpaid Federal tax liability that has been assessed, for which all judicial and administrative remedies have been exhausted or lapsed, and that is not being paid in a timely manner pursuant to an agreement with the authority responsible for collecting the tax liability.

Certification Regarding Criminal Convictions

When the proposing organization is a corporation, the Authorized Organizational Representative (or equivalent) is required to complete the following certification regarding Criminal Convictions:

By electronically signing the Certification Pages, the Authorized Organizational Representative (or equivalent) is certifying that the corporation has not been convicted of a felony criminal violation under any Federal law within the 24 months preceding the date on which the certification is signed.

Certification Dual Use Research of Concern

By electronically signing the certification pages, the Authorized Organizational Representative is certifying that the organization will be or is in compliance with all aspects of the United States Government Policy for Institutional Oversight of Life Sciences Dual Use Research of Concern.

AUTHORIZED ORGANIZATIONAL REPRESENTATIVE	SIGNATURE	DATE
NAME		

TELEPHONE NUMBER	EMAIL ADDRESS	FAX NUMBER

PROJECT SUMMARY

Overview:

Extensive research is currently underway across the University of Utah on the prediction, modeling, synthesis and characterization of a variety of material platforms that are both intellectually challenging and important to society. These studies include materials that are of particular relevance for applications in electrochemistry, high-speed computing and communications, and optics. Researchers from seven academic departments and three colleges on campus, as well as three researchers from other institutions, have already been working collaboratively. Far greater synergy can be realized if a MRSEC is established, bringing together related research and education activities under an umbrella that is broad enough in scope to include a number of diverse research activities, yet focused enough to offer a unifying theme. Formalizing these collaborative efforts will enable a greater contribution to the broader educational and outreach objectives of the University of Utah, the flagship university of the State of Utah, and to its role in the surrounding community as a leader and facilitator of advanced learning.

Intellectual Merit :

The intellectual merit of the proposed MRSEC lies in the novelty of the proposed research, with IRG leaders who have proven expertise in their respective research areas. IRG 1 will investigate hierarchical electroactive materials that allow for high conductivity, multiscale porosity for mass transport and large surface areas in electrochemical cells. The proposed collaborative IRG will utilize a combination of multiscale modeling and state-of-the-art experimental techniques to provide a fundamental understanding of the underlying correlations between structural, dynamical and electrochemical properties and phenomena operating in hierarchical electroactive structures. IRG 2 will investigate 2D and 3D Dirac materials beyond graphene. These materials exhibit high mobilities, excellent conductivity, a gapless band structure with linear dispersion and potential for high Fermi velocities, which are extremely well-suited for terahertz applications. The proposed collaborative effort will use a combination theory, synthesis and characterization of both new and currently known Dirac materials, with a special focus on topological and Weyl semimetals. IRG 3 will investigate gain-loss metamaterials and devices to optimally design PT symmetric systems, random lasers and digital metamaterials by building on powerful theories of composite materials. The proposed collaborative effort will bring to bear the mathematics of composites and nonlinear optimization to the analysis, design, characterization and fabrication of optimal gain-loss structures.

Broader Impacts :

The broader impacts lie in the new fundamental science and applications addressed by this MRSEC and its unique role in training post-doctoral fellows, graduate and undergraduate students as tomorrow?s scientists and engineers in the emerging areas of the three IRGs. Applications developed from this work will include next-generation electrochemical devices, technologies for high-speed computing and communications, integrated photonics and cancer detection. Outside the laboratory, we propose a holistic education and outreach program that extends from K-12 students to post-doctoral fellows. We intend to continue and expand some of our most successful programs from the current Center, while also introducing new programs designed to increase our overall impact. Existing programs include Science Olympiad and the REFUGES program that introduces refugees to research, while new programs include teacher training and K-12 outreach to under-represented groups through the Sorenson Multicultural Center. The Center has a strong commitment to diversity as demonstrated through gains made over the last five years in the current MRSEC. With continued emphasis on attracting well-qualified women and under-represented minorities, we expect greater diversity at all levels. The University of Utah administration and State of Utah are fully committed to the MRSEC program. In fact, the NSF 4th year review panel highlighted the extraordinary support given by the University of Utah administration. Working with the State of Utah, they provided an additional $9.5M in funds to support the current center, of which $6.5M was given for the purchase of shared facilities that included a scanning TEM, dual beam FIB, and high power THz time-domain spectroscopy system. Those shared facilities, as well as anticipated university funds for additional equipment purchases, are of critical importance to the work proposed here.

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For font size and page formatting specifications, see GPG section II.B.2.

*Proposers may select any numbering mechanism for the proposal. The entire proposal however, must be paginated. Complete both columns only if the proposal is numbered consecutively.

A. List of Participating Senior Investigators

Name	Organization	Department	Title	MRSEC Role
Ajay Nahata	***Univ. of Utah***	***Electrical Eng.***	***Professor***	***MRSEC Director***
Jeff Bates	***Univ. of Utah***	***Material Sci. & Eng.***	***Asst. Professor***	***EO&D Director***
Shelley Minteer	***Univ. of Utah***	***Chemistry, Material Sci. & Eng.***	***Professor***	***PI, IRG 1***
Scott Anderson	Univ. of Utah	Chemistry	Distinguished Professor	IRG 1 Sr. Invest.
Dmitry Bedrov	Univ. of Utah	Material Sci. & Eng.	Assoc. Professor	IRG 1 Sr. Invest.
Luca Dal Negro	Boston Univ.	Electrical Eng.	Assoc. Professor	IRG 1 Sr. Invest.
Joel Harris	Univ. of Utah	Chemistry	Distinguished Professor	IRG 1 Sr. Invest.
R. Michael Kirby	Univ. of Utah	School of Computing	Professor	IRG 1 Sr. Invest.
Valeria Molinero	Univ. of Utah	Chemistry	Professor	IRG 1 Sr. Invest.
Adri van Duin	Penn State Univ.	Mechanical Eng., Nuclear Eng., Chem. Eng.	Professor	IRG 1 Sr. Invest.
Anil Virkar	Univ. of Utah	Material Sci. & Eng.	Distinguished Professor	IRG 1 Sr. Invest.
Henry White	Univ. of Utah	Chemistry	Distinguished Professor	IRG 1 Sr. Invest.
Ilya Zharov	Univ. of Utah	Chemistry	Assoc. Professor	IRG 1 Sr. Invest.
Feng Liu	***Univ. of Utah***	***Material Sci. & Eng.***	***Professor***	***PI, IRG 2***
Vikram Deshpande	Univ. of Utah	Physics	Asst. Professor	IRG 2 Sr. Invest.
Michael Free	Univ. of Utah	Metallurgical Eng.	Professor	IRG 2 Sr. Invest.
Janis Louie	Univ. of Utah	Chemistry	Professor	IRG 2 Sr. Invest.
Ajay Nahata	Univ. of Utah	Electrical Eng.	Professor	IRG 2 Sr. Invest.
Dmytro Pesin	Univ. of Utah	Physics	Asst. Professor	IRG 2&3 Sr. Invest.
Michael Scarpulla	Univ. of Utah	Electrical Eng., Material Sci. & Eng.	Assoc. Professor	IRG 2 Sr. Invest.
Berardi Sensale-Rodriguez	Univ. of Utah	Electrical Eng.	Asst. Professor	IRG 2 Sr. Invest.
Taylor Sparks	Univ. of Utah	Material Sci. & Eng.	Asst. Professor	IRG 2 Sr. Invest.
Luisa Whittaker-Brooks	Univ. of Utah	Chemistry	Asst. Professor	IRG 2 Sr. Invest.
Heayoung Yoon	Univ. of Utah	Electrical Eng.	Asst. Professor	IRG 2 Sr. Invest.
Ken Golden	***Univ. of Utah.***	***Mathematics***	***Professor***	***PI, IRG 3***
Fernando Guevara Vasquez	Univ. of Utah	Mathematics	Asst. Professor	IRG 3 Sr. Invest.
Tsampikos Kottos	Wesleyan Univ.	Physics	Professor	IRG 3 Sr. Invest.
Yan (Sarah) Li	Univ. of Utah.	Physics	Asst. Professor	IRG 3 Sr. Invest.
Rajesh Menon	Univ. of Utah	Electrical Eng.	Assoc. Professor	IRG 3 Sr. Invest.
Keunhan (Kay) Park	Univ. of Utah	Mechanical Eng.	Asst. Professor	IRG 3 Sr. Invest.
Mikhail Raikh	Univ. of Utah	Physics	Professor	IRG 3 Sr. Invest.
Valy Vardeny	Univ. of Utah	Physics	Distinguished Professor	IRG 3 Sr. Invest.

B. Achievements under Recent NSF Support

NSF Award number DMR-1121252

Title: "MRSEC: Next-Generation Materials for Plasmonics and Organic Spintronics"
Principal Investigators: Ajay Nahata, Steve Blair and Ashutosh Tiwari
Total support: $12,000,000; Period: 09/15/2011 – 09/14/2017
Number of journal publications acknowledging this NSF award: 210
The center consists of two IRGs and an Education, Outreach and Diversity effort. In addition to the NSF funding, the center is supported by nearly $9.5M from the University of Utah and the State of Utah.

Intellectual Merit: Over the last five years, IRG1 has made significant achievements through collaborative research in THz and UV plasmonics. A theme of the former topic involved the exploration of unconventional materials for terahertz (THz) plasmonics and metamaterials. For example, we showed that liquid metals could be used to create reconfigurable plasmonic metamaterials by injecting eutectic gallium indium (EGaIn) into appropriately designed microfluidic molds [1] and then reconfigured using a variety of different techniques [2-4]. We fabricated solid metal free-standing three-dimensional metamaterials [5], by injecting liquid Ga into microfluidic molds and solidifying the metal by bringing it into contact with solid gallium at room temperature. The mold halves could then be peeled away, yielding a free-standing solid gallium structure. We used inkjet printing to create two-dimensional plasmonic and metamaterial structures in which the conductivity could be varied spatially using a combination of silver and carbon inks [6], which was used to develop unique THz filters [7] and hide images within a visually "flat" metasurface pattern [8]. We also demonstrated improved THz modulator performance using hybrid metamaterial/graphene structures [9], in which the filter resonance frequency could be adjusted by varying the graphene conductivity or number of stacked graphene layers. By introducing disorder into plasmonic structures, we demonstrated Anderson localization in the THz spectral range [10]. This observation was significant, because material losses in this spectral range have prevented studies of localization in the THz spectral range. In the UV spectral range, Al is typically the metal of choice for plasmonics. The general theme of the UV plasmonics effort has been the development of alternate materials that exhibit attractive properties for UV applications. We showed that Mg is well-suited for this spectral range and exhibits the largest localized plasmon figure of merit (FOM) in the mid- to near-UV [11]. With the introduction of an Al seed layer, Mg could be deposited with finer grain sizes, yielding smoother films. We also characterized a wide range of metal alloys and found that Mg-Al alloys exhibit a significantly improved FOM over both Mg and Al near 266 nm [12]. Ga is also known to be an appealing material for UV plasmonics efforts, but conventional vacuum deposition techniques do not allow for the creation of thin continuous films. We developed a novel method for producing continuous Ga alloy thin films that effectively match the plasmonic properties of pure Ga. The approach utilizes a standard cleanroom sputtering system and a focused ion beam machine to create UV plasmonic structures [13]. To enable UV spectroscopic applications, large area arrays of antenna structures are needed. We developed a new method for based on self-assembly and directional deposition for fabricating plasmonic nanocrescents using Al [14]. Work is ongoing to extend this capability to Mg and metal alloys.

Over the last five years, IRG2 has made significant achievements through collaborative research in organic spintronics. In the area of spin injection, we solved the problem of impedance mismatch that is encountered in traditional magnetic-electrode based injection methods [15,16]. We introduced a novel approach for generating significant inverse spin Hall effect (ISHE) signals in organic semiconductors using pulsed ferromagnetic resonance, where the ISHE is two to three orders of magnitude larger compared to continuous-wave excitation, enabling measurements in polymers that have weak spin-orbit coupling [16]. In the area of spin detection, we used the ISHE to design efficient all-electrical spin detectors [17]. Non-local Hanle devices were fabricated for manipulating spin of the carriers and used to estimate the spin lifetime of the carriers [17]. A theoretical model was developed to explain how the shape of the Hanle curve evolves upon application of an alternating current (AC) drive and its dependence upon the magnetic field magnitude and frequency [18]. We observed photocurrent enhancement in organic photovoltaic cells based on low bandgap polymer/fullerene blends by radical additives. The magnetic field-induced spin-mixing among the charge-transfer exciton spin sublevels within these devices occurred in fields up to at least 8.5 Tesla [19]. We showed how interparticle spin–spin interactions (magnetic-dipolar and spin-exchange) between charge-carrier spin pairs can be probed through the detuning of spin-Rabi oscillations [20]. We investigated the spintronic properties of organic materials that were previously not investigated for this application, as evidenced by our report of large magneto-photocurrent, magneto-electroluminescence and magneto-photoluminescence responses response in perovskite solar cells [21]. The amplitude and shape of the responses could be correlated to one another through the electron–hole lifetime. We also demonstrated an organic magnetic resonance-based magnetometer that employed spin-dependent electronic transitions in an organic diode. The device never requires calibration, operates over large temperature and magnetic field ranges, is robust against material degradation and allows for absolute sensitivities of <50 nT $Hz^{-1/2}$ [22]. Finally, we developed state-of-the-art instrumentation to perform these studies, including a scanning probe microscope for electrostatic force-based single spin detection [23].

Broader Impacts: The education and outreach effort has been extremely successful in engaging students and faculty in education, outreach and research; generating enthusiasm for science and engineering in K-12 students; and in training more undergraduate students, graduate students and postdoctoral fellows in research and developing professional skills. Broader impact has occurred at the campus level through the Center's support of a number of key programs designed to enhance diversity. As a result of Center outreach, 5634 K-12 students (3191 female, 2343 under-represented minority (URM)) participated in our programs in year five alone. The Center effort has been leveraged via collaboration with local organizations that have grown from two in the first year to 42 in the fifth year. Through the award period, our partnerships have included three local chapters of The Boys and Girls Clubs of Greater Salt Lake, elementary schools, junior high schools, high schools, three local museums, and community organizations. We partnered with the United Way and worked with our Student Advisory Committee to develop an after-school program for women, called Young and WISE (Women in Science and Engineering). This program not only introduces female high school students to materials-related science principles and applications, but also provides a mentorship component where the graduate students answer questions about applying to college and discuss issues about the workplace environment in STEM disciplines. The state of Utah had a well-established Science Olympiad program, which was on the verge of being discontinued. The Center resuscitated this program in 2011 and now coordinates both the event and volunteers. The program hosts 600-800 middle and high school students (380 female, 54 URM in 2016) each year and awards internships at the University of Utah Nanofab to the top materials science event winners. The Center also runs a week-long teacher training program each year (ASM Materials Camp) that brings approximately 25 middle school teachers onto campus during the summer to learn about materials-related topics that are relevant to middle and high school students, thereby increasing our overall impact. In addition to growing the number of programs and expanding the number of students reached each year, our REU program has become increasingly diverse and gained more visibility. The number of REU applications increased from 58 in our third year to 102 in the fifth year. In the latest applicant pool (Summer 2016), 38% of the applicants were female and 33% were URM. We made 12 offers from this applicant pool (58% females, 25% URM) with eight acceptances. This increase is due to a directed advertising campaign targeting faculty, advisors and professional organizations serving higher numbers of women and underrepresented minority students. Due to this targeted advertising, we have increased the number of qualified diverse applicants, thereby increasing the overall diversity of students admitted to the program.

The current Center has worked hard to improve diversity at all levels. Over the last five years, 46 faculty, 25 postdoctoral fellows, 63 graduate students and 26 undergraduate students, not including REU students, have been supported. The overall diversity among MRSEC participants in 2015-2016 included 28 tenure-track faculty (21% female, 7% URM), 10 post-docs (30% female, 0% URM), 34 graduate students (44% female, 6% URM) and seven undergraduate students (43% female, 14% URM). In many categories, this represents a significant gain. As an example, four of the 17 graduate students were women in year one, while 15 of the 34 graduate students were women in year five. Similarly, one of the four post-doctoral fellows was a woman in year one, while four out of the 10 post-doctoral fellows were women in year five. Also, four of the 22 faculty members were women in year one (no URM faculty), while six of the 28 faculty members were women (with two URM faculty) in year five.

Of the $9.5M in funds given by the University administration and the State of Utah, $6.5M was given for the purchase of shared facilities, including a scanning TEM, dual beam FIB and high power THz time-domain spectroscopy system. The equipment is managed by the University of Utah Nanofab and is accessible to the larger university and business community. Three faculty positions were also given to the Center and filled, in an effort to increase expertise and diversity – Luisa Whittaker Brooks (Chemistry), Berardi Sensale Rodriguez (ECE) and Heayoung Yoon (ECE) – as well as funds to augment the seed program and encourage external collaborations.

C. Introduction

The vision of the University of Utah MRSEC is to be a world-class research center that is internationally recognized in the cutting-edge research areas defined by the IRGs and a national leader in education and outreach in transmitting obtained knowledge to the broadest possible segments of society. In achieving these goals, we will train the next generation of scientists and engineers, broaden the participation of members of under-represented groups and interact with industry and transition our research into useful technology. The Center is composed of three IRGs that have clear and specific scientific goals and share common education, outreach and diversity goals. Each of the IRGs is composed of researchers with proven scientific track records in their respective areas. Under the auspices of the MRSEC, ongoing collaborations among the faculty will be strengthened and new collaborations will naturally emerge due to the interdisciplinary nature of the proposed research. The overall structure and operation of the Center will continue the most successful aspects of the existing MRSEC and incorporate new ideas, as highlighted in the proposal. The goals of the individual components of the Center are discussed below.

Controlled Hierarchical Electroactive Structures (IRG1): Next-generation electrochemical devices will demand electrodes that stably support high current densities, resulting from materials that combine facile transport of molecules, ions and electrons and high electrochemically active surface areas. Therefore, hierarchical electroactive materials are needed for most electrochemical cells that require high conductivity, multiscale porosity for mass transport and large surface areas. We will rely on strongly coupled multiscale modeling and state-of-the-art experimental techniques to provide a fundamental understanding of the underlying correlations between structural, dynamical and electrochemical properties and phenomena operating in hierarchical electroactive structures.

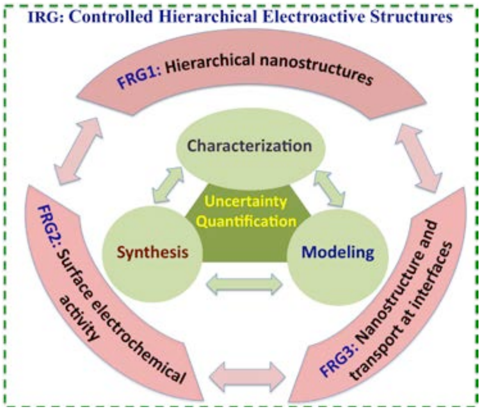
Dirac Materials Beyond Graphene for Terahertz Optoelectronics (IRG2): Next-generation technology for computing and communications will require materials that allow for control of THz radiation and enable new functionalities. 2D and 3D Dirac materials beyond graphene are ideally suited for this application given their high mobilities, excellent conductivity, gapless band structure with linear dispersion and potential for high Fermi velocities. The goal of this IRG is to understand the properties and full potential of these materials for THz optoelectronics. We will achieve this through a concerted collaborative effort involving theory, synthesis and characterization of both new and currently known Dirac materials, with a special focus on topological and Weyl semimetals.

Gain-Loss Metamaterials and Devices (IRG3): Nanostructured materials where patterns of gain and loss can be manipulated to control wave behavior are involved in critical application areas as diverse as cancer detection and integrated photonics. The objective of this IRG is to focus on Gain-Loss Metamaterials and use the power of mathematics of composites and nonlinear optimization for their analysis, design, characterization and fabrication. By building on powerful theories of composite materials, we will explore the *optimal design* of gain-loss structures in three closely related areas: (1) PT symmetric systems, (2) Random Lasers and (3) Digital Metamaterials, where the distributions of "pixels" of gain or loss in the composite nanostructure are designed, for example, to select chirality.

Education and Outreach: The mission of our Education and Outreach effort is to (1) engage students and faculty in education, outreach and research, (2) generate enthusiasm for science and engineering in K-12 students and (3) help prepare the next generation of students and postdoctoral fellows. To accomplish this mission, we intend to continue and expand some of our most successful programs, while also introducing new programs designed to increase our overall impact. Examples of these new programs include working with the Sorenson Multicultural Center in Salt Lake City to offer community education classes and services to a broad range of underrepresented groups in the Salt Lake Valley, teaching a course on Engineering Education in conjunction with the University of Utah's Center for Science and Mathematics Education and creating a new high school student research opportunity that integrates students into the high-level research problems that are currently being investigated within MRSEC.

Diversity: Over the past five years, the existing MRSEC has made notable gains in increasing diversity. Nevertheless, room for improvement exists. Over the next six years, the Center is committed to making further gains in diversity at all levels, particularly with URMs. At the faculty and postdoctoral fellow level, this will be accomplished through targeted hiring. At the graduate level, we will focus on using the REU program to encourage undergraduate students to continue their graduate studies here. Finally, at the undergraduate level, we have the potential to have the largest impact. The Salt Lake Valley is home to a large Native American population, the largest Pacific Islander population in the continental US and a rapidly growing Latino population. We will work with local community centers to interact with families in these communities, so they will know how to help their children prepare for college.

D.1. IRG 1: Controlled Hierarchical Electroactive Structures
IRG Lead: Shelley Minteer (Materials Science & Chemistry)
Senior Investigators: Anil Virkar (Materials Science), Scott Anderson (Chemistry), Ilya Zharov (Chemistry), Joel Harris (Chemistry), Mike Kirby (School of Computing), Luca dal Negro (Electrical Engineering, Boston University), Adri van Duin (Nuclear Engineering, Penn State), Dmitry Bedrov (Materials Science), Henry White (Chemistry), Valeria Molinero (Chemistry)
Other Personnel: 1 post-doctoral fellow, 10 graduate students and 5 undergraduate students
NSF Core Areas: CMMT and SSMC



Next-generation electrochemical devices will demand electrodes that stably support high current densities. High currents result from materials that combine facile transport of molecules, ions and electrons and high electrochemically-active surface areas. Therefore, *hierarchical electroactive* structures are needed for most electrochemical cells, including capacitors, batteries, fuel cells and electrolysis cells. These hierarchical material structures require high conductivity, multiscale porosity for mass transport and large surface areas. However, most electroactive structures are developed *via* a combinatorial approach of varying preparation conditions and studying the effects on the conductivity, transport, electrochemically active surface area and electrochemical response. In this IRG, we will rely on multiscale modeling and state-of-the-art experimental techniques to provide a fundamental understanding of the underlying correlations between structural, dynamical and electrochemical properties and phenomena operating in hierarchical electroactive structures. Guided by rigorous uncertainty quantification (UQ) efforts, a strongly coupled modeling-experimental approach will predict and formulate novel strategies/design rules needed for the development of controlled hierarchical electroactive structures.

This IRG will include the three Focus Research Groups (FRGs). **FRG1** will focus on the design and synthesis of hierarchical carbon-based support structures with desired morphology and size distribution of pores. These novel materials will be incorporated into FRG 2 and 3 to fabricate next-generation electrode materials. **FRG2** will focus on developing design rules for size/activity and size/stability relationships for electrocatalytic nanoparticles as well as the study of photo-assisted electrocatalysis *via* the use of plasmonics. **FRG3** will focus on understanding molecular processes occurring at charged electrode interfaces as well as understanding and fabricating optimal three-phase boundaries for electrochemical gas evolution and consumption. This knowledge will be combined with the materials design of catalysts obtained in FRG2 and the support structures of FRG1 to develop next-generation electrodes.

The Team. A highly interdisciplinary team of established experimentalists and modelers with expertise in Chemistry, Materials Science & Engineering (MSE), Electrical Engineering (EE), Nuclear Engineering (NE) and Computer Science (CS) has been assembled. Each FRG has an equal balance of modelers and experimentalists, most of whom already have an excellent track record of collaboration (20 joint publications) and extensive experience in multidisciplinary teams.

Computationally-Driven Materials-by-Design. To make significant advances in electrochemically-active interfaces, the experimental design of materials must be informed by fundamental understanding of the phenomena and processes that govern their performance. Furthermore, the nanoscale properties of materials and the quantum mechanical nature of matter enable new macroscopic properties. Where controlling the remarkable properties of matter emerging from complex correlations of the atomic and electronic constituents leads to new functionalities, modeling and simulations can provide crucial insight into these issues at a variety of scales. Our team has recently demonstrated how modeling can provide crucial guidance toward the design of advanced materials, including a rigorous *inverse design* method to engineer the shape of plasmonic particles [24], pathways to increase energy storage in supercapacitors by introduction of vacancy defects and doping with metals to recover the metallic character of graphene-based electrodes [25] and by tuning the design of nanostructured/nanoporous electrodes (pore dimensions, atomic scale surface roughness, etc.) to be commensurate with the chemical structure of the electrolyte [26-28] and the design of optimal processing conditions for the synthesis of carbon nanotubes [29].

The complexity and multiscale nature of phenomena governing the behavior of electrochemical systems often means that utilization of a single modeling technique is insufficient. The material properties and performance are often defined by a convoluted interplay between phenomena with time scales ranging from femtoseconds to seconds and length scales from Å to µm. Existing simulation and modeling approaches are incapable of accessing such broad length and time scales with fidelity at all scales. Therefore, multiscale modeling and simulation approaches that combine *ab-initio* calculations, molecular simulations, mesoscopic and continuum level modeling have to be integrated and applied to these systems. To make the multiscale modeling-guided design of complex materials a reality, the computational framework must integrate methods for uncertainty quantification (UQ) and validation and verification (V&V) with efficient parallel computations. For most of these areas, our understanding of the underlying physics is not sufficient to know *a priori* what phenomena, properties and scales are key in defining the material's/system's behavior and hence need to be captured in the multiscale modeling design. Our team has extensive experience (Molinero, Kirby, van Duin, Bedrov, Dal Negro) in development and application of this multiscale modeling approach to materials design for several complex systems including electrochemical applications.

FRG1: Controlling Hierarchical Support Structures*.*

*Ilya Zharov (Chemistry – **FRG1 Lead**), Dmitry Bedrov (MSE), Shelley Minteer (MSE/Chemistry), Luca dal Negro (EE) and Mike Kirby (SoC)*

Nanoporous carbons constitute one of the most important classes of conductive materials used in electrochemical devices, including fuel cells, electrolyzers and capacitors. They provide support of the catalytic moieties, allow for mass transport in electrochemical devices and control many of the electrical double layer properties in supercapacitors. The nanostructure of such materials plays a critical role in their performance. Therefore, the focus of FRG 1 is on novel hierarchical nanoporous carbon materials *via* experimental and computational design, preparation using templating approaches and experimental and computational characterization. We will prepare both ordered and disordered nanoporous carbon structures. The preparation of the ordered structures will be based on templating silica colloidal crystals, which will provide nanoporous materials with inverse opal structures. Utilization of nanostructured templating structures opens the possibility of introducing multiscale patterns into the designed electrode structures. The key aspect of the described approach is the precise control of the surface characteristics, morphology and composition of the carbon materials. We will also modify the surface of the nanoporous materials with amines to serve three purposes: increasing hydrophilicity of the materials for the tailoring of interfaces in FRG3, depositing metal nanoparticles for the catalytic materials studied in FRG2 and growing surface-immobilized ionomers that will introduce novel electric double layer properties studied in FRG3. The second type of nanoporous carbon material will be carbon nanofiber mats. While these materials lack order, their surface area and porosity can be controlled by the preparation conditions and their preparation from electrospun polymer fibers is a well-established process [30,31] used by the Dal Negro group. These materials will be further surface-modified to produce catalytic nanostructures for FRG2. The voids in the carbon mats will be filled with ionomers in FRG3. The above experimental work will be guided by modeling. Specifically, we will (1) perform coarse-grained simulations of colloidal particles distributions to determine how particle size of the template affects the resulting hierarchical nanostructures and (2) use ReaxFF to model the carbonization process in nanopores in order to predict the nanoscale features that can be obtained.

FRG2: Controlling Activity, Selectivity and Stability of Nanoelectrocatalysts.

*Anil Virkar (MSE – **FRG2 Lead**), Scott Anderson (Chemistry), Shelley Minteer (MSE/Chemistry), Joel Harris (Chemistry), Mike Kirby (SoC), Luca dal Negro (EE), Adri van Duin (NE), Dmitry Bedrov (MSE), Henry White (Chemistry)*

The focus of FRG2 is on materials factors that affect electrocatalyst activity, selectivity and stability. We will investigate the relationship between catalyst size and activity. Generally, activity *per* mass increases with decreasing particle size due to increasing surface area/volume ratio, but the relationship is complex and system dependent, because of the metal electronic structure and distribution of active sites [32]. The Anderson group will synthesize electrodes with size-selected atomic clusters, by mass selective deposition in ultra-high vacuum. In a recent study, Pt_n clusters deposited on electrodes [33] showed that activity increased with size from Pt_1 to Pt_4, then decreased from Pt_4 to Pt_8 and then again increased from Pt_8 to Pt_{14}. We will utilize this novel synthesis tool to investigate catalytic activity and stability of single metal clusters, bimetallic clusters, core-shell catalysts containing non-noble metal as core and platinum group metal (PGM) as shell. To further increase their catalytic performance, we will develop and implement molecular modeling tools to study these processes. We will rely on reactive molecular simulations using the ReaxFF approach. Building on the molecular and atomic scale insight, a systematic modeling and experimental study will be conducted to obtain correlations between nanostructure and electrocatalytic activity. Finally, to enable fully-reactive simulations of these electrocatalysts, we will extend the ReaxFF description of hydrocarbon catalytic reactions on metal surfaces to C/H/O species, focusing on reactions relevant to alcohol and carbohydrate oxidation catalysis. In addition, we will extend a recently developed explicit-electron concept, e-ReaxFF, to solid-state surface reactions that will enable us to include electron-transfer events within metal-surface catalysis simulations.

Loss of activity of catalysts occurs by particle growth, when there is a coupled transport of metal ions from smaller particles through liquid to larger particles with electron transport through the conducting support (*e.g.* carbon) [34,35]. We will investigate the effect of particle size distribution on the growth kinetics. Work by Popescu *et al*. [36] on Au_n clusters showed that size-selected clusters grow much slower than poly-dispersed clusters and the Anderson group has shown exceptional stability for their Pt_n clusters. We will experimentally and theoretically investigate the effect of catalyst size distribution on the growth kinetics, using the techniques described above and *in-situ* electrochemical TEM. Modeling of the coarsening kinetics will take into account the transient problem that the quasi-steady state models do not apply. This modeling and experiments will develop design rules for size/stability relationships in electrocatalytic materials.

The study of plasmonic metal nanomaterials, due to their ability to manipulate light at the nanometer scale using the phenomenon of surface plasmon resonance, has become popular. Recently, it was shown by the Minteer, Harris and Dal Negro groups that plasmonic properties can be utilized in electrocatalysis to enhance electrocatalytic selectivity and decrease catalyst passivation [37,38]. Therefore, the use of plasmonic materials as electrocatalysts provides a promising new avenue for tailoring the stability and selectivity of electrocatalysis. However, little is known about the mechanism. The current proposal aims to integrate both computational and innovative experimental synthesis and characterization in order to provide detailed understanding of the catalytic processes based on the utilization of plasmonic materials and to explore materials designs that will enable their applications.

FRG3: Nanostructure-Transport Relationships at Interfaces.

*Valeria Molinero (Chemistry – **FRG3 Lead**), Scott Anderson (Chemistry), Dmitry Bedrov (MSE), Shelley Minteer (MSE/Chemistry), Adri van Duin (NE), Henry White (Chemistry).*

FRG3 focuses on the fundamental studies of non-classical interfacial structure in complex ion- and electron-transfer processes. Specifically, the role of three-phase interfaces (gas/solid/liquid) in determining the rate of electrocatalytic reactions is at the center of these studies, in addition to ion transport in complex nanostructured architectures. Electrocatalytic reactions that generate or consume gases are the fundamental basis for many energy conversion and storage technologies [39,40]. Production of gas nanobubbles hinders H_2 and O_2 synthesis in electrolysis and disrupts electrode processes in batteries and fuel cells. Ion- and electron-transfer occurring at the three-phase boundary of individual nanobubbles of H_2, CO_2 and N_2 will be investigated by experimental and computational modeling [41-44]. Using an approach developed by the White group, single stationary nanobubbles can be maintained at disk-shaped nanoelectrodes *via* electrogeneration of gas at the three-phase boundary. Fundamental insights into gas nucleation and ion/electron transfer at the bubble interface will be investigated by the van Duin and Molinero groups using their expertise in ReaxFF simulations of interfacial reactions and coarse-grain simulations of nucleation phenomena [45-52]. Recent studies from the White group suggest that the critical nucleus of a stable bubble comprises ~1000 gas molecules. To study gas nucleation in this limit, the Anderson group will prepare electrodes decorated by size-selected Pt catalytic clusters containing with 1-60 atoms [53-55]. Air-breathing cathodes require O_2 delivery to the cathode by diffusion from a three-phase boundary [56,57]. The Minteer group will design ionomer membrane structures for forming the three-phase boundary for both biological electrocatalysts (*i.e.*, laccase enzymes) as well as metal electrocatalysts for O_2 (FRG2) deposited on mesoporous carbon architectures (FRG1). The Molinero and Bedrov groups will develop high-resolution coarse-grained molecular models of materials synthesized and investigate the relationship between transport and the nanostructure of the three-phase boundary. These models correctly represent hydrophobic and water-mediated interactions [58-60], including hydrophobic hydration and attraction [58,60-64], as well as capillary condensation [49,62,65,66] FRG3 will also focus on the coupling of ion transport and structural correlations at electrolyte/electrode interfaces developed in FRG1 for energy storage and conversion.

D.2. IRG 2: Dirac Materials beyond Graphene for Terahertz Optoelectronics
IRG Director: Feng Liu (MSE).
Senior Investigators: Vikram Deshpande (Physics), Michael Free (Metallurgy), Feng Liu (MSE), Janis Louie (Chemistry), Ajay Nahata (ECE) Dmytro Pesin (Physics), Berardi Sensale-Rodriguez (ECE), Michael Scarpulla (ECE/MSE), Taylor Sparks (MSE), Luisa Whitaker-Brooks (Chemistry) and Heayoung Yoon (ECE)
Other Personnel: 1 postdoctoral fellow, 10 graduate students and 5 undergraduate students
DMR Core Areas: EPM, CMP and CMMT

Since the discovery of radio waves in 1887, electromagnetics has played a major role in almost every aspect of our lives. For example, computing and communications have transformed science, technology, productivity and the way that we interact with one another. Such advancements have depended critically on the creation of new materials and a deep understanding of their properties. Despite this great progress, the desire for new materials remains unabated based on anticipated needs in the coming years. To understand this, we need only to look at advances in operating speeds for these two broad classes of technology over the last several decades and predictions for where they are headed. The terahertz (THz) spectral range, extending from 100 GHz to 10 THz [67], is increasingly viewed as important for these technologies and, yet, it is still often referred to as “the last frontier in the electromagnetic spectrum.” The primary reason for this lies in difficulties in creating devices that operate efficiently in this spectral range; it is too high in frequency for electronics-based approaches and too low in frequency for optics-based approaches. However, the development of new materials has the potential to deepen the impact of THz technology. A well-studied example of this is graphene, whose excellent THz properties have captured the interest of the THz community for devices that enable generation, detection and modulation of THz waves [68-74].

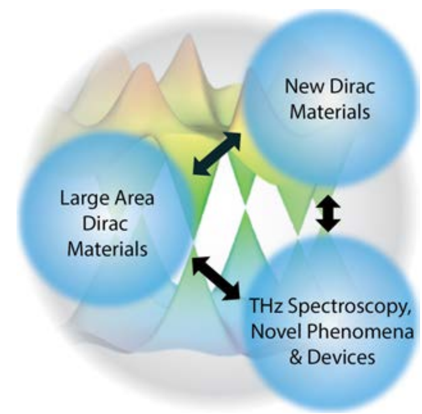


Figure 1. Synergistic research plan for the proposed IRG.

However, graphene is just one member of a wider class of largely unexplored terahertz materials that can also lead to excellent electromagnetic properties as well as rich unconventional physical phenomena. Over the past fifteen years, there has been growing interest in a novel class of materials, whose low-energy-excitation spectrum is characterized by point or line Dirac nodes with linear band dispersion [75], somewhat similar to graphene. In this IRG, we have designed a multifaceted research program that will study the interactions between THz waves and Dirac materials beyond graphene, with the goal of understanding and applying their properties to advance the state of the art in THz technology and overcome the practical materials-challenges still faced in graphene.

This IRG has three main features that make it unique:

i) It brings together a diverse and highly collaborative group of junior and senior faculty from three separate colleges, who are recognized experts in all areas of materials research that are relevant to the proposed work – theory, materials synthesis, structural/electrical characterization, THz spectroscopy and device fabrication – as noted in the synergistic research plan shown in Figure 1.

ii) The main goal of the IRG is to study topological insulators and Dirac & Weyl semimetals for their applications to THz optoelectronics. The program contains efforts in prediction, synthesis and characterization of new materials, as well as development of growth techniques for large area crystals of established materials systems. Basic science will be advanced through theoretical and experimental THz studies of transport and optical properties of 2D and 3D Dirac materials, with a special emphasis on their unique phenomenology. Thus, the proposed research encompasses great breadth and depth.

iii) The proposed work is founded on a strong basis created by the research efforts carried out by one of the IRGs in the current MRSEC, which explored the field of THz plasmonics using conventional and unconventional metals [1-8,10,76-91], including emerging materials, such as graphene [9,92-97]. All of the necessary equipment and capabilities, including significant shared facilities, are already in place.

In order to maintain efficiency and flexibility to adjust the research endeavors for a project of this size, we have divided the effort into three major tasks (Fig. 1), as discussed below.

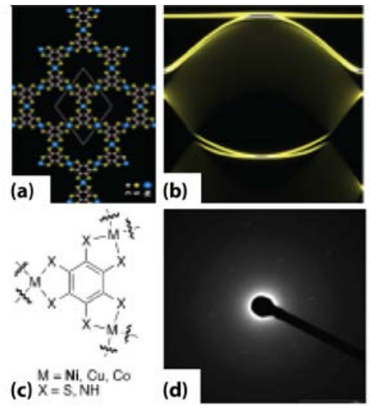


Figure 2. (a) Ball-&-stick model and (b) band structure of $Ni_3C_{12}S_{12}$ showing topological edge state. (c) Precursors of $M_3C_{12}N_{12}H_{12}$. (d) TEM image of $Ni_3C_{12}N_{12}H_{12}$.

I. New Dirac Materials: Prediction, Synthesis & Characterization *(Deshpande, Liu and Louie)* Extensive first-principles computations will be carried out to guide experiments by predicting new 2D/3D Dirac and topological materials and to help explain experiments and phenomena via the development of new theoretical approaches. One outstanding example is our recent prediction of 2D organic topological insulators (OTIs) [98-101], which led to the synthesis and preliminary characterization of a coordination polymer ($Ni_3C_{12}S_{12}$) as shown in Fig. 2 that has been identified to exhibit nontrivial topological edge states in a Dirac band [102] as well as *three new* 2D coordination polymers made of π-conjugated M_3(hexaaminobenzene)$_2$ with a chemical formula $M_3C_{12}N_{12}H_{12}$ (M = Ni, Cu, Co). These metal-organic frameworks (MOFs) are synthetically straightforward and, importantly allow for easy modification and tunability of both the metal and the ligand components. All of the materials prepared to-date display uniform thickness and are some of the thinnest synthesized MOFs known (~12 nm as measured by AFM). We propose a theory guided collaborative experimental effort towards realization of OTIs, with a special focus on studying their plasmonic properties associated with Dirac bands, calculation of the collective plasmon excitations and analysis of electron energy loss spectra (EELS) [103]. We will also systematically investigate the plasmonic properties of other 2D/3D Dirac and topological materials, in terms of band dispersion, orbital symmetry and band degeneracy. The choices of new material systems predicted will be determined in close collaboration with synthesis and characterization experiments. In addition to predicting intrinsic materials properties, we will also suggest theoretical ways to modify materials properties that are desirable for THz plasmonic applications. For example, using Bi(111) bilayer as a model system, we have shown that chemical edge modification can significantly increase the Fermi velocity of topological edge states of 2D TIs by one order of magnitude [104]. We will carry out similar theoretical studies of edge/surface modification for the new 2D/3D topological materials, including OTIs, to be tested experimentally.

II. Enabling THz Optoelectronics through Large Area Dirac Materials Synthesis. *Free, Scarpulla, Sparks, Whittaker-Brooks and Yoon*

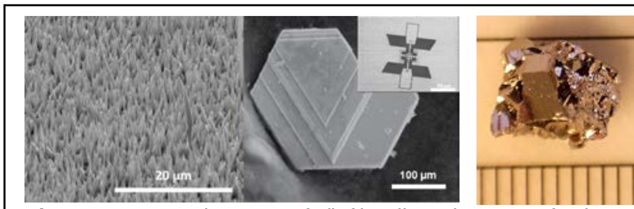


Figure 3. SEM images of (left) Aligned array of Bi2Te3 nanowires grown by vapor transport. (center) Single crystalline $BiSbTeSe_2$ platelet grown by vertical Bridgeman. (right inset) THz antenna coupled sample (scale bar 40 µm). (right) 4.5mm single crystal of Cd_3As_2.

In order to study THz interactions with the intrinsic band structure of Dirac and Weyl materials and to realize novel and high-performance THz device functionalities, samples of high quality with well-defined crystallographic alignment are required. Thus, methods of producing uniformity over the interrogated volume in terms of purity, phase and crystallographic orientation are required. This task will focus on growth methods to produce single-crystalline, oriented thin film, or nanowire array samples over areas sufficiently large to be probed either with free-space beams or with the use of antenna structures (Fig. 3). The team has already synthesized many of the topological insulators ($Pb_{1-x}Sn_xSe$, Bi_2Te_3), topological semimetals ($TaSb_2$) and Dirac & Weyl semimetals (TaP, $BiSbTeSe_2$ and Cd_3As_2, which was grown from a Cd solution - see Fig. 3). We will address the challenge of synthesizing materials with suitable dimension and orientation by conventional deposition and growth methods for single crystals, crystallographically-textured polycrystalline thin films and nanowire arrays as well as adapting novel methods such as the so-called thin film VLS [105] which can yield lateral grain sizes of hundreds of µm. Strong emphasis on characterization of the compositional, structural and electrical properties of the materials will be maintained through the project. Modifications through doping and surface adsorption will be performed to modify the THz properties and optimize the behavior of Dirac materials for a variety of applications.

III. Terahertz Spectroscopy, Novel Phenomena and Device Characterization. *Deshpande, Nahata, Pesin and Sensale-Rodriguez*

The unique band properties of Dirac materials can give rise to a wide range of novel phenomena that are important not only for fundamental science, but also a wide variety of device applications. We discuss three specific sub-topics that address this.

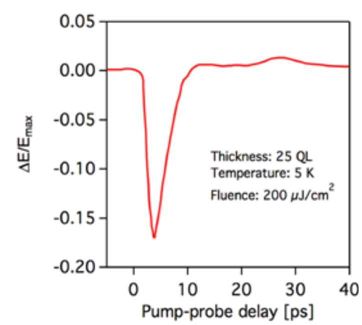


Figure 4. Normalized change in the THz electric field vs. the delay between the optical pump and THz probe for Bi_2Se_3.

THz Spectroscopy: In order to understand the behavior of charge carriers in these materials, we propose to use a combination of linear and time-resolved THz spectroscopy [106-108]. THz spectroscopy offers two important capabilities that are not easily available with other approaches: (i) it allows for direct measurement of the received THz electric field, yielding both amplitude and phase information, thereby obviating the need for Kramers-Kronig transformations [109,110] and (ii) it allows for (time-resolved) measurement of transport properties without the need for electrical contacts. Such measurements can give information about relaxation dynamics, carrier momentum scattering rates and carrier densities. In the case of 3D TIs, THz spectroscopy can be used to separate the contribution of the surface from the bulk. Real TIs are often far from ideal, because of the influence of both unintentional dopants and defects. THz measurements as a function of thickness should yield a thickness independent Drude contribution and a surface term. In Fig. 4, we show a preliminary optical pump – THz probe measurement for one specific thickness of Bi_2Se_3, a well-known TI, at low temperature. Further measurements are currently underway with this and other associated materials. In the presence of a magnetic field, Dirac materials show a range of rich phenomena [111-115]. We propose to incorporate both cryogenic temperatures and high magnetic fields into our THz spectroscopy capabilities. Finally, many of the Dirac materials discussed here are still relatively small in size. Nevertheless, we can perform both linear and time-resolved THz spectroscopy using transmission line embodiments of the system [116,117], using picosecond electrical pulses that are generated and coherently detected in close proximity. This approach only requires that crystals be larger than ~10μm x 10μm and can be deposited onto the device.

Novel Phenomena: Dirac and Weyl semimetals exhibit topological properties that manifest themselves through low-energy electron dynamics in the Dirac bands. Conventional optical experiments cannot resolve these dynamics, while the THz range is ideally suited for such studies. The best-known example of this involves Cd_3As_2. Early optical experiments in the visible-mid-infrared range placed it among conventional narrow-gap semiconductors in the 1960's, though it is now known to be a Dirac semimetal from recent ARPES [118] and transport [119] studies. On the practical side, Dirac semimetals are known to have large (metallic) Fermi velocities and high mobilities [120], making them well-suited for THz devices. Some of our focused topics include: (i) *THz tests of relativistic particle dynamics in Dirac and Weyl systems:* Weyl semimetals, as well as Dirac semimetals with mass terms forbidden by crystallographic symmetry, represent 3D analogs of graphene, since they possess 3D relativistic-like spectra. We propose to perform THz tests of relativistic dynamics in these materials; (ii) *Nonlinear optical effects in Dirac and Weyl systems:* Low doping levels and high mobility of Dirac semimetals, combined with symmetry requirements for their stability, create vast possibilities for nonlinear current responses; (iii) *Nonlocal electrodynamics of Weyl metals:* Weyl phases require breaking of either time reversal or spatial inversion symmetries, which makes them natural candidates for studies of optical activity in metallic systems [120]; and (iv) *THz studies of collective modes in Dirac systems:* Being multi-band systems, these materials can be viewed as a multi-component Fermi liquid and host many branches of collective excitations. Importantly, in Weyl semimetals, even in the absence of inter-valley scattering, different valleys are coupled to each other in the presence of a magnetic field due to the so-called chiral anomaly. This has important consequences for the observability of zero-sound-type neutral collective modes.

THz Devices: The long-term goal of investigating Dirac materials beyond graphene is to develop new device capabilities relevant to THz technology. In the case of graphene, we have significant expertise in THz device development, including amplitude modulators [121-124], phase shifters [9,92] and various metamaterials [94,125,126]. Similar device concepts will be explored for all the proposed classes of materials.

D.3. IRG-3: Gain-Loss Metamaterials and Devices
IRG Director: Kenneth M. Golden (Mathematics)
Senior Investigators: Fernando Guevara-Vasquez (Mathematics), Sarah Li (Physics), Rajesh Menon (ECE), Keunhan Park (Mechanical Engineering), Dmytro Pesin (Physics), Mikhail Raikh (Physics), Z. Valy Vardeny (Physics) and Tsampikos Kottos (Physics, Wesleyan)
Other Personnel: 1 post-doctoral fellow, 10 graduate students and 5 undergraduate students
DMR Core Areas: EPM and CMP

During the 20th century the use of composites or *metamaterials* made from two or more component materials rose dramatically. They can have effective properties not normally found in nature or which can exceed the properties of the constituents. A major factor in this rise was the development of mathematical theories of composites [127,128] yielding rigorous bounds on effective electromagnetic, thermal or mechanical properties, showing exactly what is possible given information about the mixture geometry and constituent properties. Moreover, such theories often suggest how to design microstructures, which can *attain* extremal properties. Notable benchmarks include major advances in optimal design, tomography and inversion for medical applications, photonic crystals, stealth capabilities, cloaking, and the engineering of aircraft and buildings.

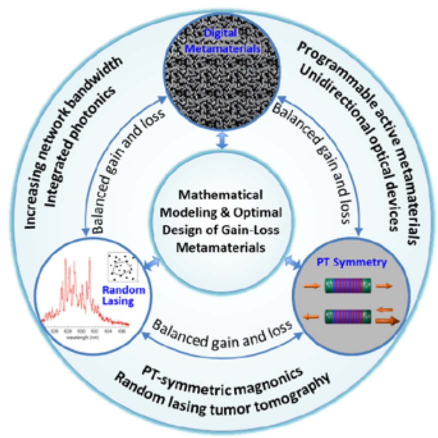


Figure 5. Clockwise from top: binary nanostructure of a Digital Metamaterial; PT Bragg grating - red and blue domains denote regions of optical gain and loss; Random Lasing spectrum in organic film.

The objective of this IRG is to bring to bear the mathematics of composites and nonlinear optimization to Gain-Loss Metamaterials (GLM), which will enable novel applications in areas as diverse as cancer detection and integrated photonics. In particular, we focus on analyzing, designing, characterizing and fabricating materials and devices where patterns of **gain** and **loss** are manipulated to achieve extraordinary wave propagation characteristics. By building on powerful theories of composites, we will explore the *optimal design* of gain-loss structures in three closely intertwined areas of application: (1) Parity-Time symmetric (PT) systems, where gain and loss must be locally balanced, (2) Random Lasers (RL) where gain and loss in random microstructures - at the critical intensity threshold - are balanced on average, or *statistically PT symmetric*, and (3) active Digital Metamaterials (DM), where we apply insights from PT and RL to enable ultra-compact active nanophotonic devices. Developing unified theoretical approaches will be facilitated by a similar Schrödinger equation formulation for both RL and PT systems. Theoretical and numerical insights will drive the design of completely novel, yet manufacturable nanophotonic devices.

Guided by the mathematics of composites, we will develop rigorous treatments of this new class of materials - GLM. Some of the exciting possible applications of our proposed work include optical diodes, PT symmetry in magnonics, high resolution random lasing tomography for early tumor detection, and DM-based chiral polarization selectors and on/off switches that drastically increase network bandwidth and power efficiency of data centers in a cost-effective and manufacturable manner. Random lasing using chiral molecules and PT systems with chiral chromophores will also be explored.

One of the distinguishing features of this IRG is the pairing of leading engineers and physicists who focus more on the experimental aspects of photonic materials and devices, with leading mathematicians who specialize in composite materials, interactions of EM waves with complex media, and optimal design of microstructures. Infusing this type of expertise will lead to investigations such as rigorous bounds on output under constraints on gain-loss nanostructure, spectral representations for output in terms of gain-loss geometry, and transitions in photonic behavior at a percolation threshold for the gain phase.

FRG 1. PT symmetric materials and structures. *Vardeny, Golden, Guevara-Vasquez, Li, Pesin and Kottos*

Introduction: Parity-Time (PT) symmetric structures in optics are devices composed of materials that may be engineered into structures having equal amount of *optical gain* and *optical loss*, based on EM wave propagation and interaction between the two parts [129]. The interplay of EM gain and loss may be designed to yield unusual optical devices [130-134] such as unidirectional optical structures, or optical diodes (see Fig. 5), laser mode manipulation in optical cavities, threshold excitation control for lasing, etc. However this concept has not been studied for magnonic propagation in ferromagnetic (FM) structures.

Research goals: This FRG is focused on: fabricating unusual PT structures in optics based on materials with large optical gain such as quantum dots, hybrid organic-inorganic perovskites and π-conjugated polymers (Golden, Li, Vardeny) that we *already have in our arsenal*; investigating PT symmetry in chiral media having optical gain (Li, Pesin, Vardeny); launching a research study of novel PT symmetry properties in *magnonics* (carried by spin-waves or magnons) (Kottos, Pesin, Vardeny); developing a theory as well as realizations of *partially PT symmetric* materials (Golden, Guevara-Vasquez, Pesin, Vardeny).

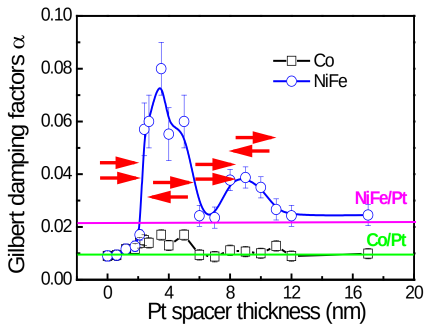


Figure 6. The damping factor in FMR of trilayers of Co/Pt/NiFe with various Pt interlayer thicknesses shows FM and anti-FM coupling caused by RKKY interaction [136] (unpublished).

***Research studies*:** In optics we will use three different structures based on materials with large, balanced gain and loss, namely PT symmetric waveguide pairs (Vardeny); PT symmetric pairs of laser resonators (Li); and PT symmetric nonlinear optics (Kottos). We will also study PT symmetric materials and devices based on chiral media, where the optical gain and loss depend on the sense of circular polarization. To achieve PT symmetry in magnonics, we first need to study magnetic materials and nanostructures that have magnetic PT symmetry properties, namely the equivalent of optical gain and loss, with control over the corresponding wave amplitude and phase. Subsequently, we will design, fabricate and characterize active structures based on the interplay between magnetic gain and loss with PT symmetric spin-wave propagation (Vardeny) based on trilayer structures [135] (FM/metal/FM), see Fig. 6. Another line of inquiry is focused on relaxing the full PT symmetry conditions and examining what happens when the system is only *partially PT symmetric*.

***Research plan*:** We plan to study a variety of optical and magnetic PT materials, choose the most suitable for engineering, then fabricate and study PT symmetric structures. In particular, for gain in magnonics we will use three techniques of launching spin-waves in FM structures. These are ps pulsed excitations that generate magnons via "electron heating" (Li); microwave pulsed excitations using FM resonance (FMR) in an external magnetic field (Vardeny); and spin-torque devices where spin-waves are generated from spin aligned carriers in metals with large spin-orbit coupling (Vardeny).

FRG 2. Interplay of gain and loss in random lasing. *Raikh, Vardeny, Golden, Pesin and Li*

***Introduction*:** Random lasers (RL) produce coherent laser emission without a traditional engineered cavity [137-138], which has been observed in solid-state disordered media [139-141], dye in cancerous tissue [142] and bones [143], etc. RL with resonant feedback was demonstrated in ZnO powder [144] and π-conjugated films by Vardeny's group [145]. The inset in Fig. 1 shows a typical RL spectrum in a film of π-conjugated polymers [145].

***Research goals*:** The aims of this FRG are four-fold: (i) Study RL near the threshold excitation (Golden, Raikh, Pesin); (ii) explore RL in gain media mixed with mirror-like scatterers that form predetermined laser resonators (Vardeny & Raikh); (iii) implement RL tomography based on the relation between the spatial ensemble-averaged RL spectra and malignant tumor morphology (Vardeny), see Fig. 3; (iv) study RL based on chiral chromophores with preferential circular polarization gain (Li, Raikh).

Research studies: (i) The spatially distributed optical gain and loss for diffusive light propagation near the RL threshold are balanced on average, and the photon density satisfies a reaction-diffusion equation. Here the spatial average of optical gain is equal to the spatial average of optical loss, but there is no local balance between them. The universality of near-threshold RL behavior manifests itself via a statistical description. An appropriate mathematical formulation should yield the eigenvalue distribution of the above equation when balanced, where the positive eigenvalues correspond to lasing conditions. In fact the eigenvalue set would fully characterize the optical response of the gain-loss system to an external excitation, treating the medium with tools borrowed from transport in polycrystalline and other composite media.

***Research plan*:** (ii) A random arrangement of nanosized mirror-like structures may lead to microcavities. The scatterers have flat boundaries that specularly reflect light, if their size exceeds the RL wavelength. When mixing such scatterers in gain media, closed loops would occur, with light trapped while travelling in loops much smaller than the light mean free path; these may serve as high-quality resonators and hence reduce RL threshold and simplify its spectrum. We plan to theoretically study and fabricate such media by mixing scatterers in a film of organic chromophores with high optical gain.

(iii) We previously established that the spatial average of the power Fourier transforms of RL spectra reveals the sizes of the underlying natural microcavities (Fig. 7) [146]. Importantly, the RL spectra based on benign human tissue impregnated with optical gain are very different than those based on cancerous tissue [144]. This may lead to an interesting application of RL in tomography, with the potential to map tumors in the human body with 1 mm^2 spatial resolution. We plan to develop this tomography in collaboration with an MD, representing the first application of RL to be commercialized.

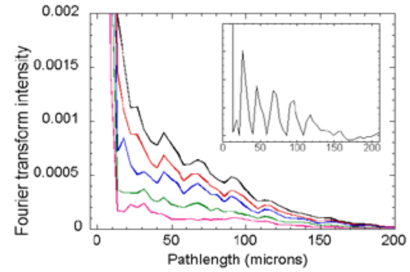


Figure 7. Average power Fourier transform (PFT) of RL emission spectra in DOO-PPV polymer film revealing equidistant cavity modes due to random resonators in the gain medium. The increased average is for 25 successive PFTs. The inset accentuates the cavity modes

(iv) We also plan to study RL in chiral media having gain that depends on the circular polarization sense; this is *terra incognita* in the RL field. This research will be based on organic chiral chromophores that we already have in our arsenal. We anticipate discovering myriad new phenomena rich in physics.

FRG 3. Active digital metamaterials for ultra-compact integrated photonics. *Menon, Guevara-Vasquez, Park and Vardeny*

Introduction: The aim of FRG3 is to exploit fundamental advances in metamaterials, optimization theory, PT symmetry and random lasing to analyze, design, fabricate and characterize active integrated photonics devices. Subwavelength control of dielectric structures has enabled novel photonic phenomena such as anomalous refraction and reflection, optical cloaking, pseudo-perfect lensing, etc. [147,148]. Recent advances in topological optimization that exploit nanofabrication have resulted in the smallest integrated passive devices ever built (Fig. 8a) [149-153].

Research goals: We will gain fundamental insights into the topology of digital metamaterials (DM). Further, by exploiting insights from PT and RL, we can expand the repertoire of DM to active or programmable integrated photonics.

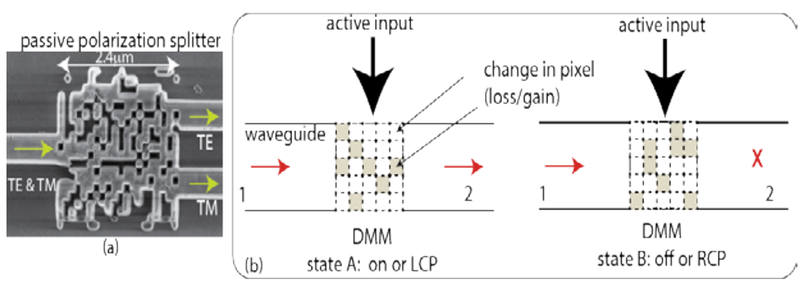


Figure 8. (a) An example of a passive DM that splits the 2 orthogonal polarizations. (b) Schematic of an active DM that can be used as a switch (ON/OFF) or a chiral polarization selector (LCP/RCP).

Research studies: We will explore two types of exemplary devices. Each device (Fig. 8b) is enabled by a unique DM designed to minimize the device area. The first is the photonic switch or modulator and the second is a chiral polarization selector that actively selects the left-circular polarized light from its right-circular polarized counterpart, and vice-versa based on an active input. Both devices will be comprised of elementary “pixels,” which contain gain or loss, whose overall distribution will be selected to maintain PT symmetry. Optimization of both devices should yield the world’s smallest version of both devices, while maximizing transmission efficiency and the ON-OFF contrast ratio.

Research plan: Guevara-Vasquez will address the theoretical question of finding bounds on the possible responses of active DM. This is innovative because most existing bounds assume passivity and ignore gain and loss phenomena. This theoretical work may also suggest novel applications to be explored by this FRG. Guevara-Vasquez will tailor optimization techniques to design such devices in an efficient and systematic manner, using gradient-based methods where possible. Menon and Guevara-Vasquez will collaborate to generate the appropriate designs, while Vardeny will provide inputs from PT symmetric concepts. Park and Menon will fabricate the devices, and Menon will characterize them.

E. Other Significant Activities

1. Education and Outreach

The mission of our Education and Outreach effort is to (1) engage students and faculty in education, outreach and research, (2) generate enthusiasm for science and engineering in K-12 students and (3) help prepare the next generation of students and postdoctoral fellows. Over the last five years, the success of the current Center in fulfilling this mission can be attributed to the strong participation of faculty, students, industrial partners, community partners and even REU students. In the next cycle, we intend to continue and expand some of our most successful programs, while also introducing new programs designed to increase our overall impact.

Community Outreach Overview: In order to maximize our contribution in community outreach, we have partnered with a number of organizations throughout the Salt Lake Valley. Examples of just a few of these partnerships include a science and engineering program offered through the University of Utah's School of Medicine, a Summer Science Festival, organized and funded by the Center and held at a local children's museum and a program called Phun with Physics, hosted by the Natural History Museum of Utah. We intend to continue these partnerships and maintain our presence in these excellent community outreach programs. We also propose to begin working with the Sorenson Multicultural Center in Salt Lake City in establishing a new program. The Center offers community education classes and services to a broad range of underrepresented groups in the Salt Lake Valley. The Salt Lake Valley is home to a large Native American population, the largest Pacific Islander population in the continental US and a growing Latino population. We plan to establish a summer program at the Center that introduces students from these communities to STEM concepts, specifically related to materials-related topics. At the end of the program, we will host a parent education night where we discuss topics including preparing and paying for college and choosing a major. There is significant existing research that shows that the earlier students and their families begin to consider college as an option, the more likely students will end up pursuing a higher education. By maintaining an ongoing presence in the Sorenson Center, we will work to encourage parents to help their children prepare to enter majors in science and engineering disciplines.

K-12 Outreach Overview: Our programs in K-12 outreach have been extremely well received. These include an after-school program at several local Boys and Girls Clubs with more than 50% under-represented minority students, the Utah Science Olympiad and teacher education programs. In addition to our active participation, we have developed modules specific to the Utah MRSEC for each of these events. During the most recent academic year, 5634 students were impacted directly by our programs at 42 different schools, including 3191 females and 2343 students from underrepresented minority groups. In terms of our direct interaction with K-12 students, there are two important benefits that we have observed. First, K-12 students learn well from our undergraduate and graduate students when they go into their classrooms, since our students help validate concepts that have already been taught in class. Second, while we believe that this interaction is of benefit for the K-12 students, it is also invaluable for our postdoctoral fellows and students. However, in many cases, our presence is not sustained. Therefore, we have also made impact through teacher education. By empowering teachers with the ability to answer questions related to science and engineering topics, we have greater impact. This will help K-12 students gain a deeper knowledge about the topics and is likely to have a more lasting impact on them.

With this in mind, we propose creating an additional program for teachers. In conjunction with the University of Utah's Center for Science and Mathematics Education (CSME), we will begin teaching a course on Engineering Education. The CSME has strong roots in the Colleges of Science and Mines and Earth Sciences and offers a Master of Science for Secondary School Teachers degree program. This program includes coursework in physics, math, chemistry, geology, geophysics and atmospheric science, but does not include any coursework in engineering. We propose adding an elective course to the program where teachers learn how engineering applies to concepts in science and consequently inspire high school students to choose materials-related majors. Such a course can highlight research topics in the Utah MRSEC, creating opportunities for faculty to interact with the teachers.

In addition to these programs, we propose to add a new high school student research opportunity to the Utah MRSEC. Over the years, a number of high school students have worked in MRSEC labs year-round and have been co-authors on high-impact publications. We propose to formalize and expand the process, with the goal of shaping how high school students think of science and engineering and getting them to consider a career in research. The program will also enable students to submit their work to national-level competitions, such as the Siemens Competition and the Regeneron Science Talent Search.

We intend to make a concerted effort to advertise the program to high schools across the Salt Lake Valley, with heavy emphasis on schools with high numbers of under-represented minority students. Unlike the REU program, this program would run year round. This program would place high school students in MRSEC labs with faculty and student mentors for 10 hours per week during the school year and full time during the summer.

Finally, we intend to continue managing the Utah Science Olympiad program. The Center took over management of the program in 2011, when it lost its previous sponsor and moved it to the University of Utah. The 2016 competition hosted approximately 600 middle and high school students from 63 schools across the state. The two gold medalists in the Materials Science event were each offered a summer internship in the University of Utah Nanofab, co-sponsored by the Center.

Undergraduate Education Overview: Our main focus for undergraduate students will be in further increasing the visibility of our REU program and on placing current University of Utah undergraduate students into MRSEC research labs. Our REU program supports approximately 10 students each year. The program has become increasingly diverse with increased visibility. We have been successful in increasing the number of quality REU applications from 58 in our 3rd year to 102 in the 5th year through strategic recruitment (all from outside the University of Utah). Of the 102 total applicants, 38% were female and 33% URM. Twelve total offers were made (58% females, 25% URM), resulting in eight acceptances. Notably, a number of these students have applied and elected to pursue graduate studies at the University of Utah each year. We will work to encourage more REU students to continue their graduate studies here.

We have supported a research program for female students in the College of Science called the ACCESS program. This program is available to freshmen women who are planning to major in STEM disciplines. In the current Center, we have funded and placed two to three ACCESS students into MRSEC labs each year. We propose to create a similar research program in the College of Engineering, funded at the same level as the ACCESS program in the College of Science, enabling new undergraduate research opportunities in MRSEC labs.

Over the past several years, we have been involved in the REFUGES (Refugees Exploring the Foundations of Undergraduate Education in Science) program administered by the Center for Science and Math Education. We are in the process of expanding Center involvement with this program. With renewed funding, Utah MRSEC can coordinate faculty to lead workshops on a number of different science and engineering topics and organize and fund training sessions in the University of Utah NanoFab for the cohort. We intend to host at least four students per academic year in MRSEC research labs.

Graduate Education Overview: We created a Student Advisory Committee (SAC) with the goal of ensuring that postdoctoral fellows and students have a formal voice in the operation and long-term success of the Center. The SAC has three members who are elected through an open election, in which all postdoctoral fellows, graduate students and undergraduate students are encouraged to vote. All three members are invited to all Executive Committee meetings and are asked for their input on all matters that come before the committee. Currently, the SAC consists of two graduate students and one undergraduate student. The SAC has been involved in a wide array of different programs, including: (1) running monthly student/post-doc meetings, which allows participants to discuss their research and bring in outside speakers who talk about topics important to them, such as professional development (2) getting student volunteers involved in Center-related outreach activities, such the Utah Science Olympiad, among others and (3) proposing and running their own activities, including a social event (Speed "Dating"), in which students and post-docs cycle through short one-on-one meetings with all participants and discuss their research and ideas for collaborations and an after-school program for high school girls (Young & WISE) that is run solely by the female graduate students in the Center. The SAC has also been charged with inviting high-profile scientists from the US and abroad to give seminars. The process of deciding whom they would like to invite has generated significant interest within the group. The SAC activities are funded based on their annual needs. They have expressed a strong interest in bringing in more guest speakers from industry, national labs and other institutions.

Mentoring is a critically important part of the educational process. It can be used as a means for enhancing the professional development of postdoctoral fellows and graduate students by providing opportunities for them to mentor others. We propose to create a mentoring program where postdoctoral fellows will be asked to formally mentor small cohorts of graduate students and graduate students will be asked to formally mentor specific undergraduate and, potentially, high school students that are part of the high school research opportunity program.

2. Diversity Strategic Plan

The current Center has worked hard to improve diversity at all levels. Diversity statistics for this last year are given in the "Broader Impacts within the Accomplishments of Recent Funding" section. At the faculty level, we improved diversity by hiring three new faculty members (Berardi Sensale Rodriguez, Heayoung Yoon and Luisa Whittaker Brooks) through positions that were given to the Center. All three faculty members are part of the "Dirac Materials beyond Graphene" IRG. At the postdoctoral fellow and graduate student level, we improved diversity through ongoing discussions with faculty about the need for greater diversity. At the undergraduate level, we improved diversity through greater visibility of our REU program at institutions with higher percentages of underrepresented minority students. As demonstrated from last year's diversity statistics, we have made encouraging gains in attracting women to join the Center, although significant room for improvement still exists. Far greater attention needs to be given to increase participation of under-represented minorities at all levels.

The MRSEC diversity plan for the next six years will work to address these issues. We look forward to receiving several additional faculty positions that will be dedicated to the Center and will be used to further enhance diversity. At the postdoctoral fellow level, we will actively recruit at major materials-related conferences as a means for attracting motivated graduates students to consider the University of Utah as a step in their career plans. For graduate students, MRSEC does not make admissions decisions directly. Therefore, we will focus on using the REU program to encourage undergraduate students to continue their graduate studies here. At the undergraduate level, we have the potential to have the largest impact. To expand opportunities for both college attendance and STEM majors to these diverse populations, we propose to establish programs in geographical areas where both the students and their parents can learn about opportunities for higher education. First-generation students face cultural barriers and many parents do not know how to help. Often, they are unaware of opportunities for both attendance and funding and students may have to leave their communities for the time they are in college. To mitigate these barriers, the focus of our outreach will not only emphasize STEM majors, but also provide information to families, so they will know how to help their children. This will be done through many of the programs listed in both the community and K-12 outreach sections.

3. Collaborations with Industry, National Laboratories and Other Sectors

Industry

- *L-3 Communications,* Salt Lake City, UT – Expertise in microwave communications systems with strong interest in developing THz communications
- *Lumos Imaging,* San Diego, CA – Start-up founded by MRSEC investigator Rajesh Menon that is commercializing computational image sensors for mobile multi-spectral imaging using metamaterials.
- *Materials and Systems Research, Inc.*, Salt Lake City, UT – Expertise in high temperature materials
- *Revalesio, Inc.*, Tacoma, WA – Collaboration to study the nucleation and stability of electrochemically generated nanobubbles
- *Simpetus Inc.,* San Francisco, CA – Expertise in cloud computing for electromagnetic simulations

National Laboratories

- *Army Research Laboratory* – Collaboration on multi-scale modeling studies
- *Center for Nanoscale Integrated Technologies (CINT),* Albuquerque, NM – Collaboration to study local carrier dynamics in nanowires
- *National Institute for Standards and Technology,* Gaithersburg, MD – Collaborations in device fabrication, analysis of localized optoelectronic properties of materials and pump-probe spectroscopy

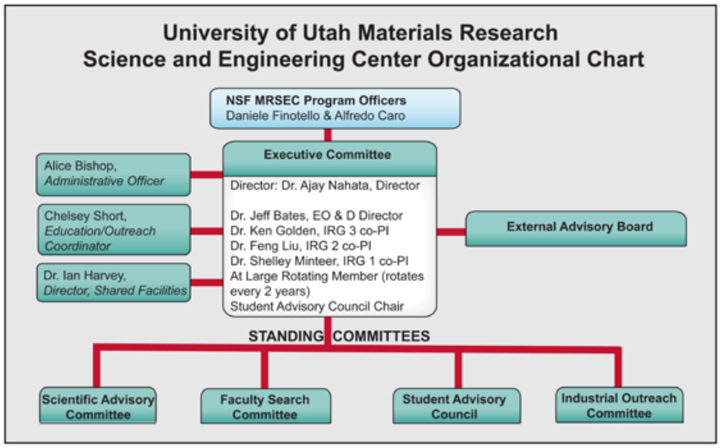
International Collaborations

- Tata Institute for Fundamental Research, India – Sushil Majumdar and S. Prabhu
- Technion, Israel – Boris Shapiro
- Tsinghua University, China – Qikun Xue
- Shanghai Jiaotong University, China – Jinfeng Jia
- University of Tokyo, Japan – Hiroshi Nishihara

- University of Twente, Netherlands – Detlef Lohse (student visiting University of Utah for 6 months)

4. Leadership, Administration and Management of the Center

Ajay Nahata (ECE) will be the MRSEC Director with overall responsibility for leadership, administration and management of the Center. He will seek counsel from President David Pershing, Provost Ruth Watkins, Vice-President for Research Thomas Parks and Associate Vice President for Research Cynthia Furse on all aspects of the Center, particularly the broader vision and implementation of the Center objectives at the institutional level. The university administration has been extraordinarily supportive of the Center, as was highlighted in the NSF fourth year review.



The Executive Committee will consist of the Director, three IRG leaders – Ken Golden (Math), Feng Liu (MSE) and Shelley Minteer (MSE & Chemistry) – the Director of Education, Outreach & Diversity (EO&D), Jeff Bates (MSE), a rotating MSREC faculty member with a two-year appointment and the chair of the Student Advisory Council. The Committee will have authority over all matters related to the operation of the Center. However, coordination of research efforts at the IRG level will primarily be the responsibility of the individual IRG leaders.

Alice Bishop will continue as the Administrative Officer for the MRSEC and oversee administrative and financial aspects of its operation. Jeff Bates will continue to work with Chelsey Short to coordinate the Education and Outreach effort. The proposed Center expects to utilize research equipment from across campus, including the significant facilities purchased by the current Center. Ian Harvey, the Associate Director of the University of Utah Nanofab, will continue as the Director of Shared Facilities.

We expect to have four committees that report directly to the Executive Committee: (1) the Scientific Advisory Committee, whose charge is to determine future research directions for the Center and oversee the MRSEC seed program, (2) the Faculty Search Committee, whose charge is to conduct searches for faculty positions given to the Center, (3) the Student Advisory Committee, which provides a formal voice for postdoctoral fellows and students in the Center and (4) the Industrial Outreach Committee, whose charge is to seek collaborative research opportunities, as well as help MRSEC participants look for commercialization opportunities for the research developed in the Center. All four committees have played an important role in the current Center. Shared governance is important to the success of such an endeavor. Therefore, members of the Executive Committee will not serve as chairs of these committees. Based on needs of the MRSEC, other committees will be created if necessary.

Each of the IRGs will hold regular monthly meetings for all participants to discuss research, exchange ideas and look for collaboration opportunities. A Center-wide meeting will be held every three months to discuss issues relevant to all MRSEC participants and to ensure transparency in all processes. We intend to convene a new External Advisory Board (EAB). The EAB will meet annually to critically assess the MRSEC objectives, research productivity and progress towards educational, scholarship and outreach goals, as well as the management of the Center. Their recommendations will be critically assessed and implemented.

An important aspect of MRSEC operation is the seed program. The Scientific Advisory Committee will oversee the seed announcement, review and selection process. We propose to follow the same general process used in the current Center. Specifically, we will fund at least three individual seed projects per year for the first three years, with each project receiving approximately $33k in direct funds for one year. Junior faculty and those from underrepresented groups (women and URMs) will be especially encouraged to apply. In years 4-6, we will gradually shift towards encouraging group proposals, where each project can receive up to $50k in direct funds for one year, with a goal of creating teams that can develop into new IRGs. All funded programs will be eligible to be competitively renewed. Proposals will be judged on a number of factors, including potential for high impact (high risk, high reward), novelty of research and potential for external funding.

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B. Appointments

2010 –	Professor, Electrical and Computer Engineering Department	University of Utah
2013 –	Associate Dean for Academic Affairs	University of Utah
2007 – 2013	Associate Department Chair, Electrical and Computer Engineering Department	University of Utah
2007 –	Adjunct Professor, Physics and Astronomy Department	University of Utah
2003 – 2010	Associate Professor, Electrical and Computer Engineering Department	University of Utah
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2002 – 2003	Visiting Scientist	NEC Laboratories America, Inc.
2000 – 2002	Scientist	NEC Research Institute, Inc.
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1992 – 1997	Graduate Research Assistant, Electrical Engineering Department	Columbia University
1992 – 1997	Consultant	AlliedSignal Inc.
1987 – 1992	Research Physicist	AlliedSignal Inc.

C. Publications

(i) Most closely related

1. Andrew Paulsen and Ajay Nahata, "K-space design of terahertz plasmonic filters," Optica **2**, 214–220 (2015).
2. Kai Yang, Shuchang Liu, Sara Arezoomandan, Ajay Nahata, and Berardi Sensale-Rodriguez, "Graphene-based tunable metamaterial terahertz filters," Appl. Phys. Lett. **105**, 093105 (2014).
3. Barun Gupta, Shashank Pandey, Sivaraman Guruswamy, and Ajay Nahata, "Terahertz plasmonic structures based on spatially varying conductivities," Adv. Opt. Mater. **2**, 565-571 (2014).
4. Z. Valy Vardeny, Ajay Nahata, and Amit Agrawal, "Optics of photonic quasicrystals," Nat. Photonics **7**, 177-187 (2013).
5. Tatsunosuke Matsui, Amit Agrawal, Ajay Nahata, and Z. Valy Vardeny, "Transmission resonances through quasicrystal arrays of subwavelength apertures," Nature **446**, 517-520 (2007).

(ii) Other significant publications

1. Jinqi Wang, Shuchang Liu, Sivaraman Guruswamy, and Ajay Nahata, "Injection molding of free-standing, three-dimensional, all-metal terahertz metamaterials," Adv. Opt. Mater. **7**, 663-669 (2014).
2. Jinqi Wang, Shuchang Liu, Sivaraman Guruswamy, and Ajay Nahata, "Reconfigurable terahertz metamaterial device with pressure memory," Opt. Express, **22**, 4065–4074 (2014).
3. Hua Cao and Ajay Nahata, "Resonantly enhanced transmission of terahertz radiation through a periodic array of subwavelength apertures," Opt. Express **12,** 1004-1010 (2004).
4. Ajay Nahata, Richard A. Linke, T. Ishi, and Keishi Ohashi, "Enhanced nonlinear optical conversion using periodically nanostructured metal films," Opt. Lett. **28**, 423-425 (2003).
5. Ajay Nahata, Aniruddha S. Weling, and Tony F. Heinz, "A wideband coherent terahertz spectroscopy system using optical rectification and electro-optic sampling," Appl. Phys. Lett. **69**, 2321-23 (1996).

D. Synergistic Activities

(1) Director, University of Utah MRSEC
(2) Editorial Board Member, *Scientific Reports* (Nature Publishing Group) 2013 – Present
(3) Co-Guest Editor, Special issue on THz Plasmonics in *New Journal of Physics*, 2013-2014
(4) Co-Organizer, *Optical Terahertz Science and Technology Conference*, March 2011
(5) Editorial Board Member of *Journal of Infrared, Millimeter, and Terahertz Waves* (Springer-Verlag) 2009 – 2014
(6) Director, Graduate Studies Committee, Department of Electrical and Computer Engineering, University of Utah 2007 – 2013
(7) Guest Editor, *Journal of Nanophotonics*, 2007– 2008
(8) External Advisory Committee Member, Engineering Physics Program, Case Western Reserve University 2005 – 2014
(9) Dekker Foundation Student Scholarship Award Selection Committee (Optical Society of America) 2005 – 2007
(10) Co-Editor, Focus Issue on Plasmonics in *Optics Express* (August 7, 2004 Issue)
(11) Developed graduate level course (ECE 6451) in Nonlinear Optics
(12) Developed graduate level class (ECE 6450) in Ultrafast Optics

KENNETH MORGAN GOLDEN – BIOGRAPHICAL SKETCH

Professor

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A. Professional Preparation

Dartmouth College	Hanover, NH	Math and Physics	B.A. 1980
New York University	New York, NY	Mathematics	M.S. 1983
New York University	New York, NY	Mathematics	Ph.D. 1984
Rutgers University	New Brunswick, NJ	Post-doc, Math	1984-1987

B. Appointments

1996 –	Professor, Mathematics	University of Utah
1991 – 1996	Associate Professor, Mathematics	University of Utah
1987 – 1991	Assistant Professor, Mathematics	Princeton University

C. Publications

(i) Most closely related

1. Adam Gully, Joyce Lin, Elena Cherkaev, and Kenneth M. Golden, “Bounds on the complex permittivity of polycrystalline composites by analytic continuation,” (issue cover) P. Roy. Soc. A-Math. Phy. **471**, 20140702 (2015).
2. Chris Orum, Elena Cherkaev and Kenneth M. Golden, “Recovery of inclusion separations in strongly heterogeneous composites from effective property measurements,” P. Roy. Soc. A-Math. Phy. **468**, 784-809 (2012).
3. N. Benjamin Murphy and Kenneth M. Golden, “The Ising model and critical behavior of transport in binary composite media,” J. Math. Phys. **53**, 063506 (2012).
4. N. Benjamin Murphy, Elena Cherkaev, Christel Hohenegger, and Kenneth M. Golden, “Spectral measure computa- tions for composite materials,” Commun. Math. Sci. **13**, 825-862 (2015).
5. N. Benjamin Murphy, Elena Cherkaev, and Kenneth M. Golden, “Anderson transition for classical transport in composite materials,” submitted, 2016.

ii) Other significant publications

1. Lyubima B. Simeonova, David C. Dobson, Olakunle Eso, and Kenneth M. Golden, “Spatial bounds on the effective complex permittivity for time-harmonic waves in random media,” Multiscale Model. Sim. **9**, 1113-1143 (2011).
2. Kenneth M. Golden, David Borup, Margaret Cheney, Elena Cherkaeva, Michael S. Dawson, Kung Hau Ding, Adrian K. Fung, David Isaacson, Steven A. Johnson, Arthur K. Jordan, Jin Au Kong, Ron Kwok, Son V. Nghiem, Robert G. Onstott, John Sylvester, Dale P. Winebrenner and Ingrid H. H. Zabel, “Inverse electromagnetic scattering models for sea ice,” IEEE T. Geosci. Remote **36**, 1675-1704 (1998).
3. Kenneth M. Golden, Stephen F. Ackley and Vicky I. Lytle, “The percolation phase transition in sea ice,”
Science **282**, 2238-2241 (1998).
4. Kenneth M. Golden, “Critical behavior of transport in lattice and continuum percolation models,”
Phys. Rev. Lett. **78**, 3935-3938 (1997).

5. Kenneth M. Golden, Sheldon Goldstein and Joel L. Lebowitz, “Classical transport in modulated structures,” Phys. Rev. Lett. **55**, 2629–2632 (1985).

D. Synergistic Activities

(1) Polar expeditions. I have traveled to the polar regions eighteen times to conduct field studies on sea ice and its role in the climate system – seven to Antarctica and eleven to the Arctic. In particular, we did experiments on the fluid and electromagnetic transport properties of sea ice, microwave backscatter experiments, as well as developed electromagnetic tomographic methods of recovering sea ice properties. I have brought many undergraduates, graduate students, and postdoctoral fellows on these expeditions to assist in the field work.
(2) Media coverage. My polar expeditions and mathematical work have been covered in over 40 newspaper, magazine, and web articles, including profiles in Science, Science News, and Scientific American. I have also been interviewed numerous times on radio and television, and featured in three videos produced by the National Science Foundation and NBC News.
(3) Scientific and general audience lectures. Given over 400 invited lectures on 6 continents, including three presentations in the U.S. Congress, many plenary and keynote addresses, as well as lectures for the general public. The general audiences have included students at elementary, junior high, and high schools, groups of undergraduate and graduate students, and business leaders. My recent public lectures have included the following: the First National Math Festival (2015) at the Smithsonian Institution in Washington D.C., a Math Encounter at the National Museum of Mathematics (2014) in NYC, the MAA-AMS-SIAM Gerald and Judith Porter Public Lecture at the Joint Math Meetings (2013) in San Diego (the largest annual mathematics meeting in the world), and the Inaugural Bernoulli Society Public Lecture at the 36th Conference on Stochastic Processes and their Applications (2013) in Boulder.
(4) Outreach and organizational service. Chair, Committee for Math Awareness Month 2009, Mathematics and Climate, Joint Policy Board for Mathematics (representing all major mathematics societies in the US); Chair, American Mathematical Society Committee on Science Policy, 2012-2013; Director of Undergraduate Studies, U. of Utah Math Dept. 2002-08; Research Experiences for Undergraduates (REU) Program Coordinator, U. of Utah Math Dept. 2003-07; Modeling Coordinator (overseeing theoretical research) for Office of Naval Research Accelerated Research Initiative on Sea Ice Electromagnetics, 1992-98, with over 60 researchers at 20 institutions; One of 12 principal investigators establishing the NSF- funded Math Climate Research Network (MCRN, https://mcrn.hubzero.org), with 12 hubs across the US, and over 100 young mathematicians funded in the program; Organized or co-organized 27 conferences, workshops, and minisymposia on the mathematics and physics of composite materials, inverse problems, sea ice, and climate change.
(5) Recognition of broader impact and knowledge transfer. 2011 Fellow of the Society for Industrial and Applied Mathematics for “extraordinary interdisciplinary work on the mathematics of sea ice”; 2013 Inaugural Fellow of the American Mathematical Society; 2014 Fellow of the Explorers Club; 2012 Myriad Faculty Award for Research Excellence (for fostering undergraduate research - I have been a research mentor to 35 undergraduates in 11 different majors, and 7 high school students), U. of Utah, $20,000; 2012 Distinguished Scholarly & Creative Research Award, U. of Utah, $10,000; 2007 University Distinguished Teaching Award, University of Utah; 1996 Member, Electromagnetics Academy; 1989 Excellence in Teaching Award, Princeton University.

FENG LIU – BIOGRAPHICAL SKETCH
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A. Professional Preparation

Tsinghua University	Beijing, China	Materials Science	B.S. 1984
Tsinghua University	Beijing, China	Solid State Physics	M.S. 1986
Virginia Commonwealth University	Richmond, VA	Chemical Physics	Ph.D. 1990
Rutgers University	New Brunswick, NJ	Post-doc, Ceramics	1991-1993
Oak Ridge National Lab	Oak Ridge, TN	Post-doc, Solid State Div.	1993-1995

B. Appointments

2007 –	Professor, Materials Science and Engineering Department	University of Utah
2011 –	Chair, Materials Science and Engineering Department	University of Utah
2007 –	Adjunct Professor, Physics and Astronomy Department	University of Utah
2002 – 2007	Director, Center for Computational Design of Nanomaterials and Nanodevices	University of Utah
2003 – 2007	Associate Professor, Materials Science and Engineering Department	University of Utah
2000 – 2003	Assistant Professor, Materials Science and Engineering Department	University of Utah
1995 – 2000	Research Scientist, Materials Science and Engineering Department	University of Wisconsin-Madison

C. Publications

(i) Most closely related

1. Zhengfei Wang, Ninghai Su, and Feng Liu, "Prediction of a Two-Dimensional Organic Topological Insulator," Nano Lett. **13**, 2842-2845 (2013).
2. Zhen Liu, Zhengfei Wang, Jiawei Mei, Yongshi Wu and Feng Liu, "Flat Chern band in a two-dimensional organometallic framework," Phys. Rev. Lett. **110**, 106804 (2013).
3. Zhengfei Wang, Zhen Liu and Feng Liu, "Quantum anomalous hall effect in 2D organic topological insulator," Phys. Rev. Lett. **110**, 196801 (2013).
4. Zhengfei Wang, Zhen Liu and Feng Liu, "Organic topological insulators in organometallic lattices," Nature Commun. **4**, 1471 (2013).
5. Miao Zhou, Wenmei Ming, Zheng Liu, Z. Wang, P. Li, Feng Liu, "Epitaxial growth of large-gap quantum spin Hall insulator on semiconductor surface," Proc. Natl. Acad. Sci. USA **111**, 14378 (2014).

(ii) Other significant publications

1. Zhengfei Wang and Feng Liu, "Self-Assembled Si(111) Surface States: 2D Dirac Material for THz Plasmonics," Phys. Rev. Lett. **115**, 026803 (2015).

2. Zhengfei Wang, Li Chen, and Feng Liu, "Tuning Topological Edge States of Bi(111) Bilayer Film by Edge Adsorption," Nano Lett. **14**, 2879-2883 (2014).
3. Miao Zhou, Zheng Liu, Wenmei Ming, Zhengfei Wang, and Feng Liu, "sd2 Graphene: Kagome Band in Hexagonal lattice," Phys. Rev. Lett. **113**, 236802 (2014).
4. Zhengfei Wang, Shou Jin and Feng Liu, "Spatially separated spin carriers in spin-semiconducting graphene nanoribbons," Phys. Rev. Lett. **111**, 096803 (2013).
5. Lizhi Zhang, Zhengfei Wang, Bing Huang, Bing Cui, Zhiming Wang, Shixuan Du, Hongjun Gao, and Feng Liu, "Intrinsic Two-Dimensional Organic Topological Insulators in Metal-Dicyanoanthracene Lattices", Nano Lett., **16**, 2072 (2016).

D. Synergistic Activities

(1) Divisional Associate Editor, Physical Review Letters
(2) Member of Editorial Board, Journal of Theoretical and Computational Nanoscience
(3) Member of Editorial Board, Open Journal of Materials Science
(4) Editor of Symposium Proceeding of 1999 MRS Spring Meeting
(5) Member of the 2006 DOE review panel for the Materials Science Program at the National Renewable Energy Laboratory-CO
(6) Member of the 2003 DOE review panel for the Materials and Engineering Physics Program at the Sandia National Laboratory-NM
(7) Co-organizer of DMP focused session of APS March meeting, 2000 & 2007
(8) Co-organizer of symposium of 1999 MRS Spring Meeting, and International Workshop on Nanostructured Materials and Interfaces, Beijing, 1999 & 2000.
(9) Four patents and six invention disclosures
(10) Developed a new course of "computational materials science---atomistic simulations" for Materials Science and Engineering majors at U of Utah.
(11) Developed a new course of "Modeling of Nanostructures on Surfaces" for Materials Science and Engineering majors at U of Utah.
(12) Reviewer for NSF, DOE, PRF and funding agencies of other countries (e.g., Canada, Australia, Singapore, China); and for more than ten journals (e.g., Nature, PRL, PR)

SHELLEY D. MINTEER – BIOGRAPHICAL SKETCH
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A. Professional Preparation

Western Illinois University	Macomb, IL	Chemistry	B.S. 1995
University of Iowa	Iowa City, IA	Analytical Chemistry	Ph.D. 2000

B. Appointments

2011 –	USTAR Professor, Chemistry and Materials Science and Engineering	University of Utah
2008 – 2011	CAS Endowed Professor of Chemistry	Saint Louis University
2005 – 2008	Associate Professor, Chemistry	Saint Louis University
2007 – 2011	Adjunct Professor, Hawaii Natural Energy Institute,	University of Hawaii-Manoa
2006 – 2007	Visiting Scholar Hawaii Natural Energy Institute	University of Hawaii-Manoa
2000 – 2005	Assistant Professor of Chemistry	Saint Louis University

C. Publications

*(i) Most closely related (undergraduate researchers noted by *)*

1. Dayi Chen and Shelley D. Minteer, “Mechanistic study of nickel based catalysts for oxygen evolution and methanol oxidation in alkaline medium,” J. Power Sources **284**, 27-37 (2015).
2. David P. Hickey, David Schiedler, Ivana Matanovic, Phuong Doan*, Plamen Atanassov, Shelley D. Minteer, and Matthew Sigman, “Predicting Electrocatalytic Properties: Modeling Structure-Activity Relationships of Nitroxyl Radicals,” J. Am. Chem. Soc. **137**, 16179-16186 (2015).
3. Fei Wu and Shelley D. Minteer, “Krebs Cycle Metabolon: Structural Evidence of Substrate Channeling,” Angew, Chem-Ger Edit. **54**, 1851-1854 (2015).
4. Nathan K. Kirchofer, Michelle Rasmussen, Frederick Dahlquist, Shelley D. Minteer, and Gui C. Bazan, “The Photobioelectrochemical Activity of Thylakoid Bioanodes is Increased via Photocurrent Generation and Improved Contacts by Membrane-Intercalating Conjugated Oligoelectrolytes,” Energ. Environ. Sci. **8**, 2698-2706 (2015).
5. Ross D. Milton, David P. Hickey, Soffiene Abdellaeoui, Koun Lim*, Fei Wu, and Shelley D. Minteer, “Rational design of quinones for high power density biofuel cells,” Chem. Sci. **6**, 4867-4875 (2015).

(ii) Other significant publications

1. Michael J. Moehlenbrock, Timothy K. Toby*, Abdul Waheed, and Shelley D. Minteer, “Metabolon Catalyzed Pyruvate/Air Biofuel Cell,” J. Am. Chem. Soc. **132**, 6288-6289 (2010).
2. David P. Hickey, Matthew McCammett, Fabien Giroud, Matthew S. Sigman, and Shelley D. Minteer, “Hybrid Enzymatic and Organic Electrocatalytic Cascade for the Complete Oxidation of Glycerol,” J. Am. Chem. Soc. **136**, 15917-15920 (2014).
3. Miao Zhang, Shuai Xu, Shelley D. Minteer, and Dana Baum, “Investigation of a deoxyribozyme as a biofuel cell catalyst,” J. Am. Chem. Soc. **133**, 15890-15893 (2011).

4. Fei Wu, Lindsey Pelster, and Shelley D. Minteer, “Krebs Cycle Metabolon Formation: Metabolite Concentration Gradient Enhanced Compartmentation of Sequential Enzymes,” Chem. Commun. **51**, 1244-1247 (2015).
5. Yang H. Kim, Elliott Campbell, Jiang Yu, Shelley D. Minteer, and Scott Banta, “Complete Oxidation of Methanol in Biobattery Devices Using a Hydrogel Created from Three Modified Dehydrogenases,” Angew, Chem-Ger Edit. **52**, 1437-1440 (2013).

D. Synergistic Activities

(1) Electrochemical Society Physical and Analytical Electrochemistry Board Member, (2005-present), Secretary/Treasurer (2007-2009), Vice-Chair (2009-2011), Chair (2011-2013)
(2) Society of Electroanalytical Chemists Board of Directors Member (January 1, 2009 – January 1, 2014), President (2015-present)
(3) Associate Editor for the Journal of the American Chemical Society (Summer 2016-present)
(4) Editorial Board of Electroanalysis (January 2012- December 2015)
(5) Technical Editor of the Journal of the Electrochemical Society (December 2011- June 2016)