COLORADO HIGHER EDUCATION COMPETITIVE RESEARCH AUTHORITY

University of Colorado:Colorado State University:University of Northern Colorado:Colorado Schools of Mines:State of Colorado

March 1, 2019

Honorable Members of the House and Senate Education Committees
State Capitol
200 East Colfax
Denver, CO 80203

Re: Annual Report of the Colorado Higher Education Competitive Research Authority (CHECRA)

Dear Representatives and Senators:

Colorado Revised Statute §23-19.7-103(3) requires the Colorado Higher Education Competitive Research Authority (CHECRA), housed at the Colorado Department of Higher Education, to report annually to the Education Committees of the Colorado House of Representatives and Senate on research projects funded by the CHECRA in the previous calendar year. This letter reports on activities and projects funded in calendar year 2018.

The CHECRA was created to provide a source of matching funds for National Science Foundation (NSF) and other competitive federal grants that require or benefit from a state match. CHECRA funding has helped to bring significant research dollars to Colorado. CHECRA spent $1.4 million in 2018 to support five multi-year research grants that jointly are bringing over $50 million in research dollars to the state. Following is a list of the multi-year research grants that received CHECRA funding in 2018:

University of Colorado (CU)

1. In 2014, the NSF awarded the University of Colorado a six-year, $22.8 million grant to continue and expand its Soft Materials Research Center into a full Materials Research Science and Engineering Center (MRSEC), one of the NSF's most prestigious awards. This Center focuses on work related to DNA nano-science and liquid crystal frontiers, an area where the University of Colorado is among the leading authorities. The CHECRA has pledged $400,000 per year for six years; 2018 was the fifth year of funding.

2. In 2016, with CU Boulder as the lead awardee, the NSF awarded a $24 million, 5-year grant for the Science and Technology Center on Real-Time Functional Imaging (STROBE). STROBE brings together universities, national laboratories, industry and international partners to create a powerful new set of real-time imaging modalities. CHECRA has pledged $400,000 for five years; 2018 was the third year of funding.

Colorado School of Mines

3. The Colorado School of Mines, along with Colorado State University, is part of the Institute for Advanced Composites Manufacturing Innovation, a consortium of 122 companies, nonprofits, universities, and research laboratories that are partnering with the federal government to create a manufacturing hub focused on U.S. leadership in next-generation materials. Approximately $2 million of this grant to the consortium is a direct financial benefit to the School of Mines. Recognizing the importance of this large initiative, as well as the number of players involved, CHECRA has pledged a limited cost share of up to $100,000 per year for five years, beginning in 2015. CHECRA made the fourth of five payments of $100,000 in 2018 to the School of Mines.

4. The NSF renewed the Colorado School of Mines' Re-inventing the Nation's Urban Water Infrastructure (ReNEWIt) Engineering Research Center, a $5.7 million grant for which CHECRA agreed to provide a continued cost share of $400,000 per year for five years. CHECRA made the third of five payments in 2018. With this grant from the NSF, the School of Mines joins leading universities in tackling acute water problems and needed infrastructure changes in the West.

Colorado State University (CSU)

5. Colorado State University received a $5.5 million Advanced Research Projects Agency-Energy (ARPA-E) grant under its rhizosphere observations optimizing terrestrial sequestration program. This work will improve predictions of soil greenhouse gas emissions and long-term carbon sequestration. CHECRA provided the second of three payments in 2018; the payment was $99,183.

In addition to the payments listed above, the CHECRA provided $500,000 for cost shares for the following Major Research Instrumentation (MRI) grants received from NSF in 2018. These grants provide higher education institutions with major instrumentation that supports the research and research training goals of the institution and are also used by other researchers regionally or nationally.

- The University of Colorado Boulder acquired a high-resolution X-ray microtomography (XRM) imaging system. This instrument is enhancing Colorado's regional abilities to image, study and design novel materials that enhance infrastructure resilience, next-generation biomedical technologies and energy production. The instrument is benefitting researchers in the broader Rocky Mountain Region as well as aiding in the training of a new generation of imaging scientists and the education and mentorship of K-12, undergraduate, and graduate students.

- Colorado State University acquired a maskless lithography system, enabling a wide range of nanoscience-related research at CSU and at neighboring institutions in the Northern Colorado/Wyoming area. Many cutting-edge areas of research in physics, engineering, chemistry and biology depend on the ability to make structures with sizes of a micron or less. This instrument is being used for research that is relevant to technology, especially solid-state electronics including magnetoelectronic (spintronics) devices, and biomedical research that are beneficial to society.

- The School of Mines acquired a Time-of-Flight Secondary Ion Mass Spectrometer (TOF-SIMS), a highly unique instrument capable of measuring and mapping chemical species at low concentrations in solid samples. The instrument is open for use on a cost-recovery basis to all academic entities in the state, and at an industrial rate to companies.

Appendices to this report include detailed information on each of the projects listed above. In addition to the millions of dollars in federal funding coming into the institutions and the state—and the impressive scientific results achieved under the projects—the research centers funded by CHECRA positively impact Colorado. As noted in the attached appendices, these benefits include support for graduate and undergraduate students, outreach to K-12 students and teachers and economic development benefits from spin-off technologies and companies.

Following are some highlights of these benefits to Colorado. We also bring to your attention Appendix A, which highlights additional benefits from the University of Colorado's projects.

- Colorado State University's work under the ARPA-E grant is promoting CSU as a drought research facility. The work with Colorado corn farmers will contribute to our knowledge of incentives that will increase drought adaptive and root enhanced maize varieties.
- The Colorado School of Mines ReNUWIt Center has continued its collaboration with the City and has a new collaboration with the Southeast Metro Stormwater Authority. In addition, ReNUWIt has an active outreach effort, including working with K-12 teachers and schools, introducing 3rd graders to water treatment, and working to support elementary school science programs and organizations such as "Girls Lead the Way."
- The School of Mines' Advance Composites Institute is exposing Colorado's intellectual and industrial resources in wind technology to a vast array of industry partners and has secured large-scale investment from industrial partners.
- The University of Colorado's STROBE project is working to realize the great opportunity this project represents for science, education, outreach to K-12 students and teachers, as well as spin-off companies and partnerships with existing local industry, universities and national labs. For example, the project provided funds to Science Discovery at CU Boulder to augment K-12 workshops for students and teachers that are delivered around the State of Colorado with emphases on reaching middle and high school teachers. STROBE is also partnering with Fort Lewis College (a non-tribal native American serving institution) to create a diverse and inclusive community that focuses on cutting edge material science.

During calendar year 2018, the Authority received a single distribution of Limited Gaming Funds of $2.1 million. Interest earnings on those funds totaled $77,325 for a total income of $2,177,325 in 2018. Expenses totaled $1,908,233.

Thank you for your support of this ongoing research. We welcome any questions.

Sincerely,

Dr. Angie Paccione
Executive Director, Colorado Department of Higher Education

Cc: Dr. Alan Rudolph, Vice President for Research, Colorado State University and Vice Chair, CHECRA
Dr. Terri Fiez, Vice Chancellor for Research, University of Colorado Boulder Colorado School of Mines
Dr. Stefanie Tompkins, Vice President for Research and Technology, Colorado School of Mines
Dr. Andrew Feinstein, President, University of Northern Colorado

Attachments:

Appendix A: Letter from University of Colorado
Appendix B: University of Colorado Soft Materials Research Science and Engineering Center
Appendix C: University of Colorado Science and Technology Center on Real-Time Functional Imaging (STROBE)
Appendix D: University of Colorado Acquisition of X-ray microtomography imaging system
Appendix E: Colorado School of Mines Institute for Advanced Composites Manufacturing Innovation
Appendix F: Colorado School of Mines Re-inventing the Nation's Urban Water Infrastructure (ReNUWIt) Engineering Research Center
Appendix G: Colorado School of Mines Acquisition of Time-of-Flight Secondary Ion Mass Spectrometer
Appendix H: Colorado State University ARPA-E
Appendix I: Colorado State University Acquisition of maskless lithography system

Research & Innovation Office
UNIVERSITY OF COLORADO BOULDER

Terri Fiez, Vice Chancellor for Research & Innovation
Research & Innovation Office (RIO)
330 Regent Administrative Center, 99 UCB
Boulder, CO 80309-0026

Terri.Fiez@colorado.edu
www.Colorado.edu/vcr
t 303 492-4499
f 303 492-5777

February 11, 2019

Mr. Spencer Ellis
Director of Educational Innovation
Colorado Department of Higher Education
spencer.ellis@dhe.state.co.us

RE: Report on 2018 CHECRA funding for the University of Colorado Boulder

Dear Mr. Ellis,

As requested, we are providing a report on CHECRA's funding for 2018. As you know, in addition to the millions of dollars in federal funding coming to the University of Colorado Boulder (CU Boulder) and the state and the impressive scientific results achieved under the projects, the research centers and projects funded by CHECRA have many additional positive benefits to Colorado. As noted in the attached appendices and in our report below, these benefits include support for graduate and undergraduate students, outreach to K-12 students and teachers, and economic development benefits from spin-off technologies and companies.

The following University of Colorado Boulder projects received CHECRA funding in the past year:

1. ***Soft Materials Research Center (SMRC)**, PI: Noel Clark* – In 2014, the National Science Foundation (NSF) awarded CU Boulder a grant to continue and expand its Soft Materials Research Center (SMRC) into a full Materials Research Science and Engineering Center (MRSEC), one of the NSF's most prestigious awards. The Center focuses on liquid crystal frontiers, an area where CU Boulder is among the leading authorities, and on work related to DNA nano-science. In 2018, the MRSEC has continued its role as CU Boulder's single most visible materials research activity nationally and internationally. <u>CHECRA has pledged $400,000 per year for six years; 2018 was the fifth year of funding</u>.
2. ***Science and Technology Center on Real-Time Functional Imaging (STROBE)**, PI: Margaret Murnane* – In 2016, with CU Boulder as the lead awardee, the NSF awarded a $24 million (5 year) Science and Technology Center (STC) grant to STROBE to build the Microscopes of Tomorrow. STROBE brings together academe (CU Boulder, UCLA, UC Berkeley, Florida International University and Fort Lewis College), national laboratories (LBL, LANL, NIST), large and small US industries, as well as international partners, to create and integrate a powerful new set of real-time imaging modalities. STROBE is developing transformative imaging modalities to create powerful and broadly-applicable real-time nano-to-atomic scale imaging modalities to address grand challenges in science and technology, while building a diverse STEM workforce. CU Boulder leads in ultrafast X-ray and visible light sources, which will enable real-time functional 3D X-ray imaging of advanced materials and advanced optical nano-imaging. <u>CHECRA has pledged $400,000 per year for five years; 2018 was the third year of funding</u>.
3. ***Acquisition of a 4D High-Resolution X-Ray Micro-Computed Tomography System for the Rocky Mountain Region**, PI: Wil Srubar III* – In 2017, the NSF awarded CU Boulder a Major Research Instrumentation grant to acquire a publicly available high-resolution X-ray tomography imaging system that will enhance CU Boulder's (and the greater Rocky Mountain Region's) ability to image, study, and design novel materials to enhance infrastructure resilience, next-generation biomedical technologies, and energy production. This project will not only advance industry, research, and institutional scientific missions and critical areas of research, including next-generation civil

infrastructure materials, biological tissues and materials for tissue repair and regeneration, natural and archival materials, smart polymers, and energy collection and storage, but it will also aid in the training of a new generation of imaging scientists and the education of K-12, undergraduate, and graduate students. CHECRA contributed $216,759 in 2018.

Additional highlights regarding the ***added benefits of each of these projects to the State of Colorado*** are described here:

1. ***Soft Materials Research Center (SMRC)***
   a. Education
      i. *Materials Science From CU (MSFCU)* – MSFCU is the Center's principal SMRC K-12 outreach activity. This program has been extraordinarily successful in reaching Colorado K-12 students with needed physical sciences presentations tuned for the Colorado curriculum. To date, over ***2,400*** classes have served ***92,500*** Colorado K-12 students, including ***75*** classes to ***2,450*** students during this reporting period. These presentations tuned specifically to fit the Colorado curriculum, provide an excellent way for Center faculty, graduate, and undergraduate students to share their enthusiasm about science with the community.
      ii. *Partnership with Arrupe High School* – In 2018, the Center worked closely with Arrupe's science teacher Stephan Graham to expand its Exploring the Nanoworld MSFCU classroom program with the new theme DNA - the Messenger. The Center-wide team (see Appendix A for list of involved postdocs, graduate students, and undergraduate students) meets regularly, developing curriculum materials including demonstrations, labs, and student handouts on the topics: introduction to natural and man-made polymers; DNA extraction; gel electrophoresis; and the societal implications of engineering new products. The team appreciated the opportunity to hone communication skills and practice conveying science topics to non-experts.
      iii. *Pathways to STEM Careers: Underrepresented Minority (URM) Undergraduates - Pathway Partnerships Program* - The Center has established research and training partnerships with three minority-serving Undergraduate Host Institutions (UHIs) having a high percentage of URM undergraduate enrollment (California State Polytechnic University, Pomona (CPP), Metropolitan State University of Denver (MSD), and California State Polytechnic University, San Luis Obispo (CPSLO)). The purpose of the initial partnership with CPP was to provide cross-disciplinary research experiences for minority undergraduate students and CPP faculty in Center laboratories, and to promote successful student projects at CPP. This program has now evolved into the Pathways Partnerships with the three UHIs above, and with a much more significant outcome metric, namely that 80% of the participating UHI undergraduate alumni, none of whom were considering graduate school before entering the program, are currently successful Ph.D. students at UCB, or have graduated with a Ph.D (see Appendix A for full list of students).
   b. Industry
      i. *Single-molecule nucleic acid sequencing using Quantum Molecular Sequencing* - Nanoelectronic DNA sequencing can provide an important alternative to sequencing-by-synthesis by reducing sample preparation time, cost, and complexity as a high-throughput next-generation technique with accurate single-molecule identification. However, sample noise and signature overlap continue to prevent high-resolution and accurate sequencing results, especially for single molecules. With a mixture of nucleotide measurements used to base call respective DNA nucleobases, it was shown that the new parameters significantly improve base calling ability over merely using LUMO and HOMO frontier orbital energies. These results have significant implications for the industrial development of a robust and accurate high-throughput nanoelectronic DNA sequencing techniques.
      ii. *Molecular-scale Photolithography of CNA and Functional Groups* - The goal of this project is molecular-scale light-directed organic synthesis to direct subsequent self-assembly of CNA

and DNA on a surface. We expect in the coming year to demonstrate molecular-scale additive manufacturing of organic species capable of sequence-directed assembly of nano-devices on a solid substrate.

2. ***Science and Technology Center on Real-Time Functional Imaging (STROBE)***
   a. Education
      i. The STROBE Research and Education Team came together to design and submit a successfully-funded grant for a Partnership in Research and Education for Materials (PREM) for Functional Nanomaterials. Professor Ryan Haaland from Fort Lewis College (FLC) led the PREM proposal - a strong partnership between FLC, Norfolk State University (NSU) and STROBE. This collaboration integrates education and research across FLC (a non-tribal Native American Serving Institution), NSU (a member of the Historically Black Colleges and Universities), and STROBE. The goals for PREM are to create a diverse and inclusive community that focuses on cutting edge material science that explores the multi-scale interplay of atomic and meso-scale structure and emergent physical phenomena; exciting applications that attract a diverse group to STEM; novel and effective curricula and pathways that recruit and retain the best in STEM; and long-term assessment to improve strategies and share best practices. This resulted in a $3.6M PREM grant from NSF over 6 years. STROBE is funding a joint postdoctoral scientist shared between CU Boulder and FLC to enhance the undergraduate physics laboratories at FLC to attract and retain more students to STEM fields.
      ii. STROBE successfully received supplemental funding to support additional undergraduate students and teachers at FLC and Boulder.
      iii. STROBE and CHECRA funds are supporting ≈20 students, postdoctoral scientists and staff in Colorado.
      iv. STROBE is providing funds to Science Discovery at CU Boulder to augment K-12 workshops for students and teachers that are delivered around the State of Colorado, with particular emphases on reaching middle and high school teachers and students in the four-corners region.
      v. STROBE is offering unique professional development opportunities for students in project and people Management and Leadership that are not usually offered to students in the Physical Sciences, and are attracting non-STROBE participants.
      vi. New transdisciplinary graduate programs in imaging science are now available at CU Boulder, to better prepare students for the 21st century workplace, with students already enrolled.
   b. Industry
      i. NIST Boulder laboratories is using technologies developed by the Boulder STROBE PIs (commercialized through KMLabs).
      ii. STROBE industry members Ball Aerospace (Boulder) and Cymer-ASML (San Diego) are providing funds for student professional development and innovation competitions.
      iii. STROBE is developing methods to characterize samples provided by Intel, Ball, IMEC, IBM and elsewhere that are challenging to characterize using other techniques. These bring many opportunities for students for internships, permanent positions and for knowledge transfer.
   c. Other
      i. STROBE nodes at Boulder (Murnane, Raschke, Hernandez-Charpak, Kapteyn) and UCLA (Musumeci, Miao) developed an NSF Major Research Infrastructure (MRI) proposal for a multimodal hybrid photon-electron functional imaging system, to allow for an unprecedented functional multi-scale characterization of complex samples. We are very happy that this proposal was funded at ≈$3.3M, as it will allow STROBE to develop new hybrid imaging concepts.
      ii. A diverse set of 26 graduates were hired by US National Laboratories and Industries.
      iii. Colorado students and faculty won many prizes, awards and fellowships.
3. ***Acquisition of a 4D High-Resolution X-Ray Micro-Computed Tomography System for the Rocky Mountain Region***
   a. Education

i. *Direct Student Training and Mentorship* – The project is supporting the education, training, and mentorship of a new generation of advanced instrumentalists for Colorado, who will establish a regional expertise in high-resolution imaging of both hard and soft materials. A multitude of graduate research assistants (GRAs) and postdoctoral research associates (PRAs), have had the unique opportunity to aid in the installation, training, and operation of the XRM. The GRAs and PRAs have been actively involved in establishing the supporting physical infrastructure that is required to run the XRM as a part of an instrument core facility. More explicitly, the GRAs and PRAs have aided in website development, software development (for internal/external services, reservations, trainings, and billing), as well as data management strategies and solutions for the large-file data that are generated by this instrument.

ii. *Student Outreach and Teaching Activities* – This instrument is being planned for use during regular outreach activities (often involving our PI team) with the Society for Women Engineers and the CEAS Building Opportunity through Leadership and Diversity (BOLD) program to attract top, diverse students. Expert Users utilize the proposed instrument to perform activities, such as "Imaging Insect Cuticles" to excite students about relationships between mechanics and structure during BOLD's "Student for a Day" and "Explore Engineering Days." This instrument will be used to develop 'hands-on' lab modules to enhance interactive learning, made possible by the ease of disseminating XRM images and analysis in ImageJ or Matlab. Due to unprecedented growth in the College of Engineering and Applied Science (CEAS), this XRM will engage a large number of students through instrument room tours, demonstrations, and the ability to test materials specific to each course or student project. Many students (100's-1000+/year) will benefit from the XRM. We are developing modules to relate material structure to function in Mechanical of Materials in both Civil (CVEN 3161; >150 students/year; taught by Srubar, Hubler) and Mechanical Engineering (MCEN 2063; >250/year; Ferguson) and develop new lab modules for Measurements and Data Analysis (MCEN 3047; >250/year; Stoldt). Expert Users will be working with teaching assistants or student project teams in design/capstone courses. Project co-PIs Bryant, Ferguson, and McLeod will develop a new upper division course on Bioprinting using Additive Manufacturing.

b. Industry

i. The XRM is a publicly available resource being leveraged to advance the scientific missions of industry partners throughout the Rocky Mountain Region.

Reports on our three CHECRA-funded projects are attached.

We are very appreciative of CHECRA's support for the University of Colorado Boulder. Thank you for this important support.

Sincerely,

DocuSigned by:
Terri Fiez
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Terri Fiez
Vice Chancellor for Research & Innovation
CU Boulder Research & Innovation Office

Attachments (3): Appendix A, Appendix B, Appendix C

cc: Victor Bright
Colisse Franklin
Hallie Adams

NSF award to University of Colorado, Boulder (UCB)
NSF Award DMR-1420736 (Previously DMR-0820579)
Title: Soft Materials Research Center
Period of Performance: 11/1/14 – 10/31/20
Total 2018 CHECRA Funding: $400,000/ Total CHECRA Grant: $400,000 per year for 6 years
Award PIs: Noel A. Clark, David M. Walba, Christopher N. Bowman, Jennifer N. Cha

SUMMARY

The Liquid Crystal Materials Research Center (LCMRC or the Center) has existed on the University of Colorado – Boulder campus since the early 1980s, with block funding from the NSF Division of Materials Research since September 1993. The LCMRC is currently funded as an NSF Materials Research Science and Engineering Center (MRSEC), one of an elite national network of advanced materials research programs.

DESCRIPTION OF THE PROJECT, PRINCIPAL PERSONS OR ENTITIES INVOLVED IN THE PROJECT

A major theme of materials science as we enter the 21st century is understanding and manipulation of the interactions between self-organizing complex molecules. It is precisely here that the study of liquid crystals has the greatest impact. Nowhere else are the requirements for under- standing the delicate interplay between molecular architecture and its macroscopic manifestations more demanding than in the directed design of liquid crystals.

The Liquid Crystal Materials Research Center is one of the principal centers of liquid crystal study and expertise in the world, its research spanning the range from cutting-edge, basic liquid crystal and soft materials science to the development of enhanced capabilities for commercially important electro-optic, nonlinear-optic, chemical, biological, and other novel applications. The Center is a unique venue worldwide for research on key aspects of liquid crystal science and technology, chief among these the science and application of ferroelectric liquid crystals. The core Center research program is at the University of Colorado, Boulder.

The Center's research is organized within an Interdisciplinary Research Group addressing three major project themes: 1) understanding the relationship between molecular structure and macroscopic materials structure and properties of liquid crystals; (2) inventing new and useful ways of controlling liquid crystal behavior through interaction with surfaces; and (3) inventing and exploring new polymer materials possessing unique properties deriving from liquid crystallinity. Each of these research themes integrates *molecular modeling and design, chemical synthesis, physical studies,* and *applications development* into a multidisciplinary, collaborative research effort.

In 2018, the CHECRA funding was allocated to the three focus areas of the center described in this summary – research, industrial outreach, and education outreach.

FUNDING ALLOCATED TO EACH PRINCIPAL PERSON OR ENTITY

Research

The past year of MRSEC, with NSF funding supplemented by the CHECRA matching state funds, has continued in its role as CU Boulder's single most visible materials research activity nationally and internationally. A summary of major research accomplishments is as follows:

New Generation of Clickable Nucleic Acids Exhibit Improved Binding and Specificity to Complementary DNA - Center researchers have synthesized a second-generation CNA polymer that is one atom shorter compared to the first generation CNA. This challenge required the development of a novel synthetic strategy that will find use in the general preparation of eneamides, a previously difficult to obtain reactive moiety. These nucleobase monomers react via radical thiol-ene polymerization to furnish oligomers with an internucleobase spacing in line with that of DNA, and as a result, the second generation CNA is capable of binding to DNA in a sequence specific manner. The resulting duplex is stable enough that it can be resolved by polyacrylamide gel electrophoresis. Moreover, a single basepair mismatch greatly diminishes the binding of the polymer, demonstrating that the polymer is exquisitely sensitive to sequence composition. The foremost impact of these results is the development of a synthetic nucleic acid analog that binds to complementary native strands of DNA in low salt and mixed aqueous/organic conditions. This enables the Center to generate materials of higher ordered self-assembled structures that employ the specificity of intermolecular interactions both for their formation and for subsequent function. Furthermore, in contrast to previous protected monomers, these recently developed, acetyl-protected monomers do not inhibit radical reactions, permitting strategies for rapid, sequence specific oligomerization via sequential additions.

•***A Reentrant Isotropic Phase*** – An azobenzene-core chiral mesogen designed for a photoactive ferroelectric liquid crystal system with switchable polarization displays a highly unusual phase sequence, with a re-entrant, optically isotropic, fluid phase found below smectic phases in mixtures with high enantiomeric purity. The re-entrant isotropic phase is found on the basis of X-ray scattering and freeze-fracture transmission electron microscopy experiments not to be a cubic or other highly ordered phase but instead a translationally disordered liquid. Remarkably, the peak position of this short-ranged ordering indicates a molecular spacing of ~30Å, much shorter than the molecular length. The material also forms a gel under a wide range of concentrations in 50:50 ethanol/chloroform solutions. Ultraviolet/visible and infrared spectroscopy and quantum chemistry calculations suggest that the primary unit in the re-entrant isotropic and gel phases is a dimer composed of molecules crossed by about 90°, which hinders the formation of crystal phases and forms tubules of helical aggregates in the gel phase.

•***Influence of electrostatic interactions in the atomistic molecular dynamics simulation of liquid crystals*** – The influence of force field details in all-atom molecular dynamics (MD) simulations on the predicted thermodynamic, structural, and dynamic properties of bulk 4-cyano-4′-pentylbiphenyl (5CB) systems have been investigated in the 292–368 K temperature range. The effect of the molecular dipole moment and the details of dihedral potential for biphenyl unit were investigated using both polarizable (POL) and non-polarizable (NP) versions of the quantum chemistry-based force field. The POL predicted densities for the nematic and isotropic phases of bulk 5CB were found to be in excellent agreement with available experimental data. The nematic-isotropic transition temperature (TNI) showed strong sensitivity to the force field details, MD simulations with partial atomic charge distributions and molecular dipole moment corresponding to high-level quantum chemistry calculations predicted an overestimation of the TNI by about 30 K. Rescaling the charges to allow the molecular dipole to be closer to experimentally reported values of 5CB dipole in condensed phases, significantly improved the prediction of TNI as well as other thermodynamic and dynamic properties of 5CB, showing that induced dipoles must be included in MD simulations of LCs.

•***Aptamer Displacement by Ligands and Complementary DNA*** - DNA nanotechnology exploits Watson-Crick base-pairing to engineer a variety of nanoscale structures and processes with applications ranging from biosensing to molecular computing. Strand-displacement DNA reactions involve an exposed single-strand overhang known as a "toehold" to initiate the reaction between a DNA duplex and a competitive strand that ultimately replaces the toehold-bearing strand via a mechanism known as branch migration. The use of functional DNA sequences, such as aptamers (which bind non-DNA ligands) in strand displacement reactions has the potential to interface DNA nanotechnology with a wider array of chemical signals. We employed single-molecule tracking in conjunction with Förster Resonance Energy Transfer to study the displacement of a DNA aptamer from a surface-immobilized oligonucleotide by complementary DNA or by the ligand to which the aptamer was designed to bind. We found that the ligand actively disrupted the DNA duplex in a similar manner to the complementary DNA in the presence of a toehold. Interestingly, the ligand-displacement kinetics was intricately connected to the details of the exposed toehold; in particular it required the partial exposure of the aptamer's binding site. These findings provide initial design rules for the incorporation of functional DNA-ligand systems into DNA nanotechnology strand-displacement platforms.

• ***Effect of a Polymerizable Tail System on the Mesogenic Properties and Cross-Linking of Mono-Imidazolium-Based Ionic Liquid Crystal Monomers*** - We demonstrate that an ether-based n-alkoxy-2,4- hexadiene polymerizable tail system is an effective and modular alternative to traditional ester-based polymerizable tail groups (i.e., acrylate, methacrylate, sorbate) and alkyl-1,3-diene tails for the design of radically polymerized ionic liquid crystal (ILC) monomers. Several series of nonsymmetric 1-vinylimidazoliumbromide- based ILC monomers containing these different polymerizable tail systems were synthesized and compared for their ability to form thermotropic liquid crystal (TLC) phases and to be photocross-linked with TLC phase retention. The n-alkoxy-2,4- hexadiene tail system was found to be more favorable/conducive to TLC phase formation than acrylate, methacrylate, and sorbate tails. It was more similar to the alkyl-1,3-diene tail system in terms of its more favorable effect on TLC behavior; however, it is more modular/easier to synthesize, more resistant to thermal Diels–Alder side reaction, and more isomerically pure, making it better for ILC monomer design. Also, the n-alkoxy-2,4- hexadiene tail system was found to be very amenable to radical photo-cross-linking with TLC phase retention. To demonstrate this feature, an example cross-linkable ILC monomer with this tail system was synthesized and polymerized in the smectic A TLC phase, and the monomer and polymerized material were characterized for their ionic conductivity behavior.

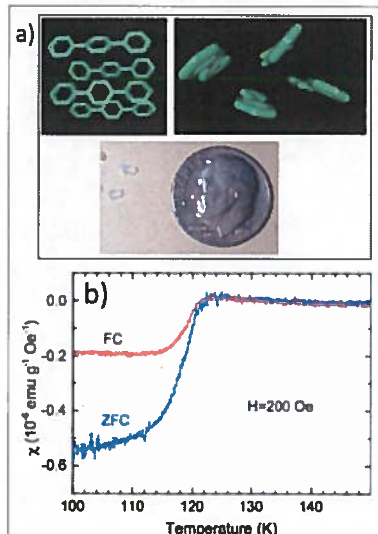

Figure: Crystal structure of undoped paraterphenyl and single crystals. Na doped crystals exhibit magnetic susceptibility changes indicative of a Meissner effect at T = 120K.

•***Seed - Dynamic Characterization of Soft, Tunable Hydrogels*** - We seek to develop experimental/analytical methods for assessment of viscoelasticity (i.e., conformational changes in the polymer chains) and poroelasticity (i.e., fluid flow through the porous network) in hydrogels at small length scales (i.e., nm to µms). We will develop hydrogels possessing viscoelastic, poroelastic, or visco-poroelastic behavior first using ionic hydrogels [developed with input from S. Bryant (UCB

Chemical & Biological Engineering) and Devatha Nair (UC Anschutz Medical Campus School of Dentistry], and then using hydrogels based on homopolymers of a single nucleobase or homopolymers of specific repeating nucleobase sequence. Time-dependent characterization across multiple length (nm to μm) scales will be carried out via state of the art dynamic AFM (with the DelRio group at NIST). Our multifaceted approach with cross-disciplinary expertise will provide new and validated methods to assess the complex properties of hydrogels with applicability to many soft materials. We are uniquely positioned to make key contributions to the measurement science, standards, and technology of soft, tunable hydrogels, aimed, in particular at how their chemistry dictates properties and then how their properties can be optimized to perform specific engineering applications (e.g., tissue engineering, sensors, actuators, wound healing, etc.).

•***Seed - High Temperature Superconductivity in Organic Solids*** - The highest achieved superconducting critical temperature for an organic material at standard pressure is 33 K, observed in the alkali-doped fullerene RbCs2C60; with nonfullerene organic superconductors the transition temperatures are of order 10 K or less. A recent report claims superconductivity above 120 in paraterphenyldoped with potassium, as suggested by a clear diamagnetic signal beginning at 120 K, interpreted as the superconducting Meissner effect [R.-S. Wang et al., arXiv:1703.05804]. However, absence of zero resistance in transport measurements makes the claim of superconductivity questionable. This result is nevertheless exciting, both for the physics as well as the potential for even higher Tc values. We have been able to grow and study by AFM the electronic structure of single terphenyl crystals, exploring the electronic states filled by the doping and characterizing their energetics by angle resolved photoemission. This project will apply the extensive expertise on the UCB campus in organic crystal growth and characterization, and capabilities for the study of the electronic structure and transport properties of electronic materials to explore a variety of alkali-doped polyphenylenes for superconductivity. In any case, thepolyphenylenes appear to be an exciting new organic electronic system.

• ***Seed - "Redhouses" Enhanced Photosynthesis and Crop Production in Greenhouses with Scalably Manufactured Energy-converting Optical Metamaterials*** - This seed project extends the development of functional polymer photonics at large scale beyond its initial applications in radiative cooling to biotechnology application, seeking new directions and possibly a new center thrust for Scalable Manufacturing of Nanostructured Functional Soft Matter. Tremendous interdisciplinary application spaces exist as UCB by leveraging its traditional disciplinary strength in physics, chemistry, ecology, and multiple sectors of engineering. This proposal aims to develop a transformative greenhouse technology, a "Redhouse" with 50% more photosynthesis light at no additional energy cost using nanostructured optical metamaterials as greenhouse envelope materials for high-yield crop production.

Rapid Construction of a Step-Growth Polymer with Dynamic Pendant Functionalities - In an effort to improve the polymer chain length of CNAs, we have explored the possibility of creating a 'blank slate' polymer onto which pendant functionalities can be later introduced. To this end, we developed the *Scheme* below, a highly efficient, atom-economic, and inexpensive polymerization between divinyl sulfone and *tert*-butylcarbazate, which yields a polymer with more than 60 repeat units, alternating between sulfone and Boc-protected hydrazine moieties. After unveiling the hydrazine functionality, we can install a wide variety pendant groups, including phenyl, furan, pyrrole, pyridine, and nucleobase functionalities, all of which are derived from available aldehydes. Moreover, these pendant groups can undergo dynamic exchange with solution-phase aldehydes, which could enable the rapid construction of polymer-scaffolded dynamic combinatorial libraries.

DNA-Assembled Core-Satellite Upconverting-Metal Organic Framework Nanoparticle Superstructures for Efficient Photodynamic Therapy - This work reports the DNA-mediated assembly of core-satellite structures composed of Zr(IV)-based porphyrinic metal-organic framework (MOF) and $NaYF_4$,Yb,Er upconverting nanoparticles (UCNPs) for photodynamic therapy (PDT). MOF nanoparticles (NPs) generate singlet oxygen ($^1O_2$) upon photoirradiation with visible light without the need for additional small molecule, diffusional photosensitizers such as porphyrins. Using DNA as a templating agent, well-defined MOF-UCNP clusters were produced where UCNPs were spatially organized around a centrally located MOF NP. Under NIR irradiation, visible light emitted from the UCNPs was absorbed by the core MOF NP to produce $^1O_2$ at significantly greater amounts than what could be produced from simply mixing UCNPs and MOF NPs. The MOF-UCNP core-satellite superstructures also induced strong cell cytoxicity against cancer cells, which were further enhanced by attaching epidermal growth factor receptor (EGFR) targeting affibodies to the PDT clusters, highlighting their promise as theranostic photodynamic agents.

Synthesis and Assembly of Click Nucleic Acid Containing PEG-PLGA Nanoparticles for DNA Delivery - delivery of both chemotherapy drugs and siRNA from a single delivery vehicle can have a significant impact on cancer therapy due to the potential for overcoming issues such as drug resistance. However, the inherent chemical differences between charged nucleic acids and hydrophobic drugs have hindered high yield entrapment of both components within a single carrier. We demonstrate here that significant encapsulation of nucleic acids is achieved within PLGA containing polymers by incorporating the use of click nucleic acids. First, CNAs were incorporated into a triblock copolymer of poly-(ethylene glycol)-b-CNA-b-lactic-co-glycolic acid (PEG-CNA-PLGA) from which polymer nanoparticles were generated. The CNA-containing polymer particles encapsulated high loadings of DNA complementary to the CNA sequence whereas PEG-PLGA alone showed minimal DNA loading. Furthermore, the dye pyrene could be successfully co-loaded with DNA in the polymer particles as well as a complex, larger DNA sequence that contained an overhang of DNA complementary to the CNA.

<u>Industrial Outreach</u>

Single-molecule nucleic acid sequencing using Quantum Molecular Sequencing - Nagpal and coworkers, have develop a new single-molecule nucleic acid sequencing method using a high-throughput nanoelectronic method called Quantum Molecular Sequencing. Nanoelectronic DNA sequencing can provide an important alternative to sequencing-by-synthesis by reducing sample preparation time, cost, and complexity as a high-throughput next-generation technique with accurate single-molecule identification. However, sample noise and signature overlap continue to prevent high-resolution and accurate sequencing results, especially for single molecules. Probing the molecular orbitals of chemically distinct DNA nucleobases (Ade nine A, Guanine G, Cytosine C, Thymine T) offers a path for facile sequence identification, but molecular entropy (from nucleotide conformations) makes such identification difficult when relying only on the energies of lowest-unoccupied and highest-occupied molecular orbitals (LUMO and HOMO). Here, nine biophysical parameters were developed to better characterize molecular orbitals of individual nucleobases, intended for single-molecule DNA and other nucleic acids (like CNA) sequencing using quantum tunneling of charges. For this analysis, theoretical models for quantum tunneling were combined with transition voltage spectroscopy to obtain measurable parameters unique to the molecule within an electronic junction. Scanning tunneling spectroscopy was then used to measure these nine biophysical parameters for the different nucleotides in DNA, and a modified machine learning algorithm identified nucleobases. With a mixture of nucleotide measurements used to base call respective DNA nucleobases, it was shown that the new parameters significantly improve base calling ability over merely using LUMO and HOMO frontier orbital energies. Furthermore, at different pH conditions, and hence reversible perturbation of nucleic acid chemistry, extremely high accuracies for identifying DNA bases were observed with a confusion matrix (high true positive and extremely low false positive and negative calls). These results have significant implications for the industrial development of a robust and accurate high-throughput nanoelectronic DNA sequencing techniques.

Molecular-scale Photolithography of CNA and Functional Groups - The goal of this project is molecular-scale light-directed organic synthesis to direct subsequent self-assembly of CNA and DNA on a surface. We first utilize optically written azobenzene monolayers to orient liquid crystal polymers that create a new form of optical mask using the Barry Pancharatnam phase to modulate both the polarization and phase of the optical field. Singularities in this optical field are projected into a flow cell (b) where dark nulls of arbitrarily small size enable top-down patterning of molecular monolayers. Feasibility tests with standard photoresist demonstrate 10-fold violation of the diffraction limit (c). We are now integrating two photosensitive monolayer chemistries into the system including a photolabile cyclooctyne (d) and NPPOC protected nucleobases. We expect in the coming year to demonstrate molecular-scale additive manufacturing of organic species capable of sequence-directed assembly of nano-devices on a solid substrate.

<u>*Education Outreach*</u>

The Center carries out a variety of education and outreach activities that aim to enhance science literacy and achievement in communities ranging from the general K-12 population to its undergraduate and graduate students. Highlights from the past year include:

•***Materials Science From CU (MSFCU)*** - The Center plans to continue Materials Science from CU, its principal SMRC K-12 outreach activity. This program has been extraordinarily successful in reaching Colorado K-12 students with needed physical sciences presentations tuned for the Colorado curriculum. To date over ***2,400*** classes have served ***92,500*** Colorado K-12 students, including ***75*** classes to ***2,450*** students during this reporting period. These presentations tuned specifically to fit into the Colorado curriculum, provide an excellent way for Center faculty, graduate, and undergraduate students to share their enthusiasm about science with the community.

•***Partnership with Arrupe High School*** – During 2018, the Center worked closely with Arrupe's science teacher Stephan Graham to expand its Exploring the Nanoworld MSFCU classroom program with the new theme DNA - the Messenger. The Center-wide team [post-doc Dylan Domaille (IRG2, Chem E), graduate students Albert Harguindey (IRG2, Chem E), Sam Goodman (IRG2, Chem E), Elizabeth Delesky (IRG2, Chem E), Kate Macri (IRG1 Chemistry), Alyssa Martinez-Finkle (IRG1, Chemistry), Mike Tuchband (IRG1, Physics) and undergraduate Valerie Toman (Chemistry, Metro State University)] meet regularly, developing curriculum materials including demonstrations, labs, and student handouts on the topics: introduction to natural and man-made polymers; DNA extraction; gel electrophoresis; and the societal implications of engineering new products. The team appreciated the opportunity to hone communication skills and practice conveying science topics to non-experts.

•***Pathways to STEM Careers: Underrepresented Minority (URM) Undergraduates*** - *Pathway Partnerships Program* - The Center has established research and training partnerships with three minority-serving Undergraduate Host Institutions (UHIs) having a high percentage of URM undergraduate enrollment: •California State Polytechnic University, Pomona (CPP), •Metropolitan State University of Denver (MSD), and •California State Polytechnic University, San Luis Obispo (CPSLO). The purpose of the initial partnership with CPP was to provide cross-disciplinary research experiences for minority undergraduate students and CPP faculty in Center laboratories, and to promote successful student projects at CPP. This program has now evolved into the Pathways Partnerships with the three UHIs above, and with a much more significant outcome metric, namely that 80% of the participating UHI undergraduate alumni, none of whom were considering graduate school before entering the program, are currently successful Ph.D. students at UCB, or have graduated with a Ph.D.: •Angel Martinez in the SI Smalyukh group in Physics, now a postdoctoral researcher in the Penn MRSEC; •Alyssa Martinez-Finkle, Eduardo Guzman, Lee Foley, Alicia Gamble in the SI Walba group in Chemistry & Biochemistry. •James Amarel, •Nicholas Kuehl, •Mitch Magrini, and •Vincent Nguyen are currently undergraduates in the program. Another Partnership student, •Carlos Guerra, is currently employed as a research technician before continuing on to graduate studies. • Julia Blackmon (MSD) and • Dania El-Batal (MSD) have been admitted into the 2018 REU Program.

The successful establishment of these Pathways is the result of recognizing and focusing on key elements of training, mentoring, and evaluation. The elements that have been applied overall are now summarized, although it should be noted that not all of them may apply to any given student:

Recruiting and Evaluation – Recruiting is carried out at the UHI by UHI faculty, who seek qualified undergraduate minority students interested in pursuing an REU experience. Selected students begin their research in the UHI labs in the context of the joint UHI/UCB research activities of the program, with student and advisor receiving funding from the program. The following summer, the students continue with an REU at UCB, working on the same or a related project, and pursue this further after returning to the UHI. The longer-term continuity of the research activity promotes a much deeper commitment to research by the student and allows a more in-depth evaluation of the student's abilities than is possible after a typical REU. Students may return for a second UCB REU, and in one case the student was hired as a Professional Research Assistant after graduating from the UHI and before becoming a graduate student. Students interested in graduate school and perceived to have the potential for successfully pursuing graduate-level research are encouraged to apply to graduate schools, including UCB. In the case of UCB, the student's research achievements and the faculty experience with him or her in the program are considered, enabling the student to gain either full or provisional graduate admission.

Mentoring – Once at UCB, the academic strengths and weaknesses of each UHI student are assessed and an academic program structured accordingly. The CPP students have performed well in their class-work and Ph.D. Candidacy exams, with assistance ranging from none in some cases to an intense mentoring plan including homework tutoring in others.

Research – The UHI students have become valued members of their respective research teams, having published, or on track to do so. UHI students are supported at UCB by Research Assistantship funds from MRSEC and other sources, or by departmental Teaching Assistantships. The Pathway Partnerships program demonstrates directly an effective strategy for facilitating the transition from undergraduate to graduate STEM training of capable URM students who find themselves on academic trajectories that would not otherwise have afforded such an opportunity. In order to encourage faculty participation, the Center has started SMRC Diversity Fellowships, which provide 0.5 year of RA support to Center SIs for a UHI or other URM student.

Pathway Partnership with Metropolitan State University of Denver (MSD) - The Center has formalized a Pathway Partnership with Metro State University of Denver, an urban university with a large URM undergraduate population. This partnership is based on the research collaboration between Prof. Ethan Tsai, an Assistant Professor in the MSD Department of Chemistry and Center graduate, with the group of Center SI D. Walba. During the academic year Tsai trains and prepares students at his lab at MSD. Research projects extending over several AYs and summers will enable evaluation and involvement of students, which, in this case, will be enhanced by the proximity of the Center (only 30 min from MSD). During the current reporting period MSD alumni Alicia Gamble and Lee Foley are now advancing to candidacy in their graduate work as PhD students in the UCB Department of Chemistry. MSD Students Julia Blackmon and Dania El-Batal began their Center research careers as REUs in June 2018.

NSF award to University of Colorado, Boulder (UCB)
NSF Award: 1548924
Title: Science and Technology Center on Real-Time Functional Imaging (STROBE)
Period of Performance: 10/01/2016 – 09/30/2021 ($24M over 5 yrs pending satisfactory progress)
Total 2017 CHECRA Funding: $400,000
Award PI's: Margaret Murnane, Jianwei Miao, Rafael Piestun, Markus Raschke, Naomi Ginsberg

Project Overview:

Microscopic imaging is critical for discovery and innovation in science and technology, accelerating advances in materials, bio, nano and energy sciences, as well as nanoelectronics, data storage and medicine. Fortunately, all areas of imaging, from electron to visible to X-ray, are undergoing revolutionary advances. However, no imaging technique can address a critical question underlying much of science and technology in the 21st century: how local (nanoscale) and extended (mesoscale) structure and interactions determine the properties and function of a material or biological system. Opaque, scattering and disordered samples common in chemistry, materials, and biology present a formidable challenge using any imaging modality. Notable demonstrations aside, current X-ray, electron, and optical microscopies are simply too slow to routinely image functioning systems in real space and time. This severely limits progress in science and technology.

The NSF STC on Real-Time Functional Imaging (STROBE) is addressing this challenge by integrating different imaging modalities with underpinning technologies – advanced algorithms, fast detectors, big data manipulation and hybrid/adaptive imaging. Unlike conventional approaches - where scientists develop different, stand-alone, imaging technologies to solve specific problems – STROBE is integrating different imaging modalities with electrons, X-rays and optical nanoscopy to develop transformative imaging modalities that address grand challenges in science and technology. In essence, STROBE is building the Microscopes of Tomorrow.

The Vision of STROBE is to transform imaging science and technology of functioning nano-systems. The Mission of STROBE is to create powerful and broadly-applicable real-time nano-to-atomic scale imaging modalities to advance imaging science and increase access that can be used to address grand challenges in science and technology, while building a diverse STEM workforce. STROBE's goals are to:

- Develop a new set of powerful, broadly applicable, accessible real-time imaging modalities using electrons, X-rays and light that can image disordered systems, implement dynamic imaging with a large field of view, with chemical and magnetic contrast, with atomic/molecular/nanoscale resolution. We are pushing each imaging mode to its fundamental limits and integrating them to reach beyond these limits.
- Address key challenges common to all imaging modalities: the need for more powerful image deconvolution algorithms, THz to X-ray and electron sources, fast/sensitive detectors, spectrally/spatially/temporally shaped electron/X-ray/light illumination fields, and the need to manipulate and visualize large data sets.
- Educate a diverse group of students for innovative STEM careers in the 21st century. Imaging science is inherently multidisciplinary, spanning computing, physics, engineering, materials, nano and bioscience. STROBE is developing new multidisciplinary degree and professional development/entrepreneurship programs, with international and industrial collaborations.

- Develop and assess best practices for broadening participation in STEM by implementing long-term programs designed and optimized for under-represented groups: women, Native American, Hispanic and African American students.
- Engage in multiple modes of knowledge transfer with industry, national labs, other scientists and the public.

Project benefits to the state of Colorado (Include support for graduate and undergraduate students, outreach to K-12 students and teachers, spin-off technologies and companies):
STROBE brings several benefits to the State of Colorado and is very cognizant of the great opportunity this project represents for science, education, outreach to K-12 students and teachers, as well as spin-off companies and partnerships with existing local industry, universities and national labs. In the first 15 months of STROBE, the following activities benefitted the state –

- The STROBE Research and Education Team came together to design and submit a successfully-funded grant for a Partnership in Research and Education for Materials (PREM) for Functional Nanomaterials. Professor Ryan Haaland from Fort Lewis College (FLC) led the PREM proposal - a strong partnership between FLC, Norfolk State University (NSU) and STROBE. This collaboration integrates education and research across FLC (a non-tribal Native American Serving Institution), NSU (a member of the Historically Black Colleges and Universities), and STROBE. The goals for PREM are to create a diverse and inclusive community that focuses on cutting edge material science that explores the multi-scale interplay of atomic and meso-scale structure and emergent physical phenomena; exciting applications that attract a diverse group to STEM; novel and effective curricula and pathways that recruit and retain the best in STEM; and long-term assessment to improve strategies and share best practices. This resulted in a $3.6M PREM grant from NSF over 6 years, for which we are delighted. STROBE is funding a joint postdoctoral scientist shared between CU Boulder and FLC to enhance the undergraduate physics laboratories at FLC to attract and retain more students to STEM fields.
- STROBE nodes at Boulder (Murnane, Raschke, Hernandez-Charpak, Kapteyn) and UCLA (Musumeci, Miao) developed an NSF Major Research Infrastructure (MRI) proposal for a multimodal hybrid photon-electron functional imaging system, to allow for an unprecedented functional multi-scale characterization of complex samples. We are very happy that this proposal was funded at ≈$3.3M, as it will allow STROBE to develop new hybrid imaging concepts.
- STROBE successfully received supplemental funding to support additional undergraduate students and teachers at FLC and Boulder.
- STROBE and CHECRA funds are supporting ≈20 students, postdoctoral scientists and staff in Colorado.
- NIST Boulder laboratories is using technologies developed by the Boulder STROBE PIs (commercialized through KMLabs).
- STROBE is providing funds to Science Discovery at CU Boulder to augment K-12 workshops for students and teachers that are delivered around the State of Colorado, with particular emphases on reaching middle and high school teachers and students in the four-corners region.
- STROBE industry members Ball Aerospace (Boulder) and Cymer-ASML (San Diego) are providing funds for student professional development and innovation competitions.
- STROBE is offering unique professional development opportunities for students in project and people Management and Leadership, that are not usually offered to students in the Physical Sciences, and are attracting non-STROBE participants.

- New transdisciplinary graduate programs in imaging science are now available at CU Boulder, to better prepare students for the 21st century workplace, with students already enrolled.
- STROBE is developing methods to characterize samples provided by Intel, Ball, IMEC, IBM and elsewhere, that are challenging to characterize using other techniques. These bring many opportunities for students for internships, permanent positions and for knowledge transfer.
- A diverse set of 26 graduates were hired by US National Laboratories and Industries.
- Colorado students and faculty won many prizes, awards and fellowships.

2018 STROBE Highlights (STROBE.colorado.edu):

The STROBE team has been extremely productive, publishing >41 papers in top journals, while students and faculty received >33 major awards and presented >200 invited/plenary/keynote talks all over the world. We are particularly excited by the many collaborations between STROBE members at different nodes, with our 19 industry and 15 national laboratory collaborators, as well as strong joint grant and IP products. Finally, STROBE students and postdocs are in high demand, with >26 hires by universities, industry and national labs - the vast majority of these within the US.

STROBE Colorado Publications from 2018 (STROBE.colorado.edu):

1. Dynamic 2D implementation of 3D diffractive optics, H. Wang, R. Piestun, Optica 5, 1220 (2018).
2. Nanoimaging and Control of Molecular Vibrations through Electromagnetically Induced Scattering Reaching the Strong Coupling Regime, E.A. Muller, B. Pollard, H.A. Bechtel, R. Adato, D. Etezadi, H. Altug, M.B. Raschke, ACS Photonics 5, 3594 - 3600 (2018).
3. Compressed sensing FTIR nano-spectroscopy and nano-imaging, B. ästner, F. ähling, A. Hornemann, G. Ulrich, A. Hoehl, M. Kruskopf, K. Pierz, M.B. Raschke, G. übbeler, C. Elster, Optics Express 26, 18115 (2018).
4. Adaptive wavefront shaping for controlling nonlinear multimode interactions in optical fibres, O. Tzang, A.M. Caravaca-Aguirre, K. Wagner, R. Piestun, Nature Photonics 12, 368 - 374 (2018).
5. Single-shot 3D coherent diffractive imaging of core-shell nanoparticles with elemental specificity, A. Pryor, A. Rana, R. Xu, J.A. Rodriguez, Y. Yang, M. Gallagher-Jones, H. Jiang, K. Kanhaiya, M. Nathanson, J. Park, S. Kim, S. Kim, D. Nam, Y. Yue, J. Fan, Z. Sun, B. Zhang, D.F. Gardner, C.Sato Baral Dias, Y. Joti, T. Hatsui, T. Kameshima, Y. Inubushi, K. Tono, J.Yang Lee, M. Yabashi, C. Song, T. Ishikawa, H.C. Kapteyn, M.M. Murnane, H. Heinz, J. Miao, Scientific Reports 8, (2018).
6. Far Infrared Synchrotron Near-Field Nanoimaging and Nanospectroscopy, O. Khatib, H.A. Bechtel, M.C. Martin, M.B. Raschke, L. Carr, ACS Photonics 5, 2773 - 2779 (2018).
7. Y. Esashi, C.T. Liao, B. Wang, N. Brooks, K. Dorney, C. Hernández-García, H. Kapteyn, D. Adams, M. Murnane, "Ptychographic amplitude and phase reconstruction of bichromatic vortex beams", Optics Express 26, 34007 (2018).
8. C. Bevis, R. Karl, J. Reichanadter, D. Gardner, C. Porter, E. Shanblatt, M. Tanksalvala, G. Mancini, Henry Kapteyn, M. Murnane, D. Adams, "Multiple beam ptychography for large field of view, high throughput, quantitative phase contrast imaging," Ultramicroscopy 184, 164-171 (2018).
9. R. Karl, G. Mancini, D. Gardner, E. Shanblatt, J. Knobloch, T. Frazer, N. Hernandez-Charpak, B. Mayor, M. Tanksalvala, C. Porter, C. Bevis, D. Adams, H. Kapteyn, M. Murnane, "Full-Field Functional Imaging of Nanoscale Dynamics Using Tabletop High Harmonics", Science Advances 4, eaau4295 (2018).

NSF award to University of Colorado, Boulder (UCB),
NSF Award: 1726864
Title: MRI: Acquisition of a 4D High-Resolution X-Ray Micro-Computed Tomography System for the Rocky Mountain Region
Total 2018 CHECRA Funding - $216,759
Award PI's – Wil V. Srubar III, Mija H. Hubler, Robert R. McLeod, Stephanie J. Bryant, Virginia L. Ferguson

Summary: This Major Research Instrumentation award to acquire a high-resolution X-ray microtomography (XRM) imaging system is advancing a broad spectrum of research that is of particular interest to the State of Colorado. This instrument, which is capable of imaging through materials in 4D, is enhancing our regional abilities to image, study, and design novel materials that enhance infrastructure resilience, next-generation biomedical technologies, and energy production. More specifically, the instrumentation is advancing critical research areas, including next-generation civil infrastructure materials, biological tissues and materials for tissue repair and regeneration, natural and archival materials, smart polymers, and energy collection and storage. The instrument is also benefitting researchers in the broader Rocky Mountain Region, as well as aiding in the training of a new generation of imaging scientists and the education and mentorship of K-12, undergraduate, and graduate students through synergistic outreach activities

Project Description and Principal Personnel Involved:
This project is being led by Professors Wil Srubar, Ginger Ferguson, Bob McLeod, Mija Hubler, and Stephanie Bryant in the College of Engineering and Applied Science. The goal of this project is to acquire, install, and operate a high-resolution, X-ray micro-computed tomography (XRM) system with in situ mechanical loading, temperature-controlled testing, and time-resolved (4D) imaging capabilities that will become a vital resource for the greater Rocky Mountain Region.

A ZEISS Xradia 520 Versa was acquired by the University of Colorado Boulder and officially installed in December 2017. A unique paring of X-ray source and objective turret enables the ZEISS XRM to achieve unparalleled resolution (700 nm) and phase contrast in both small and large (300 mm) samples. A mechanical testing kit was included that permits in situ imaging of material behavior in 3D/4D under controlled temperature, compression, and tension, enabling previously unobservable deformation and failure. Specifically, the ZEISS Xradia 520 Versa system includes a 160 kV high-energy micro-focus X-ray source and staging platform, a 2kx2k high-resolution 16-bit CCD digital camera assembly, a ZEISS 0.4X large field of view (FOV) camera assembly, a ZEISS high contrast, low resolution 4X detector, a ZEISS high contrast, ultra-high resolution 20X detector for high energy and 4-axis tomography, a motorized precision sample stage with a load capacity of 15kg and 360° capability, automatic filter changer with 12 standard filters, a radiation-safe four-door steel enclosure with redundant safety interlock, temperature control, and "X-ray On" indicator light, and interior camera. The system comes with alignment and calibration standards for quality control. The In Situ Interface Kit for the Xradia 520 Versa is complete with a CT5000- RT in situ tension-compression stage with a normal speed gear (0.1 mm/min to 1.0 mm/min) and a 5kN max load. The Kit includes a Deben CT5000-TEC in situ Healing/Cooling and Tension/Compression Stage in which compression and/or tension tests can be carried out during X-ray scanning, with external user-controlled actuation. Tests can also be carried out at specified temperatures. The loading grips can be modified to perform flexural or indentation testing. Two (2) dedicated computer workstations for the XRM instrument operations and post-processing and 3D image reconstruction were also acquired. An advanced imaging software package, Dragonfly Pro, provides a common workspace for multi-scale (nm to cm) correlative microscopy with a simple user interface.

The acquisition of the ZEISS Xradia 520 Versa has been disseminated both formally and informally to parties of interest (both internal and external to the University of Colorado Boulder). Public announcements have been made through campus media outlets, college- and department-level communications, as well as e-mail announcements to colleagues at colleges and universities in the Rocky Mountain Region (e.g., Colorado School of Mines, Montana State University, South Dakota School of Mines and Technology).

Benefits to the region: As a publicly available resource, the XRM is being leveraged to advance the scientific missions of industry, individual researchers, and research institutions throughout the Rocky Mountain region. Annual working group meetings and a biannual materials imaging symposium are facilitating dissemination of state-of-the-art imaging science, enabling continuous recruitment of new users, and catalyzing new local and regional collaborations.

The project is also supporting the education, training, and mentorship of a new generation of advanced instrumentalists for Colorado, who will establish a regional expertise in high-resolution imaging of both hard and soft materials. A multitude of graduate research assistants (GRAs) and postdoctoral research associates (PRAs), have had the unique opportunity to aid in the installation, training, and operation of the XRM. The GRAs and PRAs have been actively involved in establishing the supporting physical infrastructure that is required to run the XRM as a part of an instrument core facility. More explicitly, the GRAs and PRAs have aided in website development, software development (for internal/external services, reservations, trainings, and billing), as well as data management strategies and solutions for the large-file data that are generated by this instrument. The project has enabled the education, training, and mentorship of a new generation of advanced instrumentalists, who are establishing a regional expertise in high-resolution imaging of both hard and soft materials.

In addition to direct student training and mentorship, the XRM will be serving in student outreach and teaching activities. This instrument is being planned for use during regular outreach activities (often involving our PI team) with the Society for Women Engineers and the CEAS Building Opportunity through Leadership and Diversity (BOLD) program to attract top, diverse students. Expert Users utilize the proposed instrument to perform activities, such as "Imaging Insect Cuticles" to excite students about relationships between mechanics and structure during BOLD's "Student for a Day" and "Explore Engineering Days." We are planning to use this instrument to develop 'hands-on' lab modules to enhance interactive learning, made possible by the ease of disseminating XRM images and analysis in ImageJ or Matlab. Due to unprecedented growth in the College of Engineering and Applied

Science (CEAS), this XRM will engage a large number of students through instrument room tours, demonstrations, and the ability to test materials specific to each course or student project. Many students (100's-1000+/year) will benefit from the XRM. We are developing modules to relate material structure to function in Mechanical of Materials in both Civil (CVEN 3161; >150 students/year; taught by Srubar, Hubler) and Mechanical Engineering (MCEN 2063; >250/year; Ferguson) and develop new lab modules for Measurements and Data Analysis (MCEN 3047; >250/year; Stoldt). Expert Users will be working with teaching assistants or student project teams in design/capstone courses. Finally, co-PIs Bryant, Ferguson, and McLeod will develop a new upper division course on Bioprinting using Additive Manufacturing.

Institute for Advanced Composites Manufacturing Innovation (IACMI)
Colorado School of Mines (Mines)
CHECRA Grant: $100,000 (per year for 5 years)
Reporting Period: January 1 - December 31, 2018

Summary:
IACMI's Wind Turbine Technology project focuses on lower the levelized cost of wind energy while simultaneously increasing the quality and reliability of wind turbines. To this end, the project has several targets:

1) Decreasing mold cycle time
2) Integrating thermoplastic matrices into the current production process
3) Augmenting the robustness of fabric placement through automation
4) Conducting in-press nondestructive evaluations (NDE)

The main focus of the team at Mines this past year was to contribute to the first two targets in the project, but advances were also made in the area of NDE (item 4). More specifically, the CY2018 contributions made by the Mines team made several key contributions to the goal of the wind technology area. The contributions can be summarized in three main areas:

1) Generation and delivery of a database of mechanical properties (tension, compression, shear, fatigue) that benchmarks the performances of the new thermoplastic fiber reinforced composites against the industry status-quo thermoset composites.
2) Integration of the model for the kinetics of free radical polymerization of thermoplastic resins that was developed and delivered in CY2017 into NDE methodologies.
3) Fundamental evaluation of the adhesive properties of 4 different binders (2 thermoset, 2 thermoplastic) in their ability to be used to join segments of wind turbine blades together. The fracture toughness data generated by Mines informed the selection of the adhesive used to join the 13 m wind turbine blade together that is being made in CY2019.

Description of the project, the principal persons or entities involved in the project, and the amount of funding allocated to each principal person or entity:

Replacing thermoset with thermoplastic matrices in fiber reinforced composites used to construct wind blades offers the promise of reducing the levelized cost of electricity (LCOE). Thermoplastic use facilitates the end of service life recycling thus providing opportunities to create manufacturing jobs in the conversion of the reclaimed materials. The potential ability of thermoplastics to reduce the manufacturing cycle time strongly affects LCOE and therefore provides the strongest incentive for their commercial adoption. Naturally, for thermoplastic composites to be utilized, the mechanical properties must be equivalent to thermosetting composites.

Principal Senior Investigators	**Funding from CHECRA**
Aaron Stebner	$100,000

The manner in which each principal person or entity applied the funding in connection

with the project
$34,632: Summer Salary + Fringe for PI Aaron Stebner and Co-I Joe Samanuik

$540: Supported PhD student Peter Caltagirone stipend

$25,428: Supported administrative assistant Amy Brice to assist in facilitating the management of the research program.

$41 supported researchers to travel in-state for in-person collaboration with the National Wind Technology Center

$2,041 was spent on experiment supplies

$4,256: supported Post Doc Yasuhito Suzuki, PhD students Dylan Cousins and Peter Caltagirone, and PI Aaron Stebner to travel to IACMI meetings in Detriot, MI (Jan 2018), and Cousins + Caltigirone to travel to the summer meeting in Knoxville, TN (Jul 2018)

$5,355: went to indirect costs

$27,707: supported the procurement of a plasma pen and microscope to support the research activities

Results achieved

1. **Mechanical testing of thermoplastic panels**
A vast number of mechanical tests were conducted to qualify the final selected Elium resin system and various fiber layup geometries, in duplicates of at least 5, and then repeated for an epoxy resin system that is used in today's wind turbine blades. In total, over 3,000 individual mechanical tests were conducted for the four fiber layups (*i.e.*, $[0/0/0/0]_2$ from 0 degree, $[0/0/0/0]_2$ from 90 degree, $[0/90/90/0]_2$ from 0 degree, and $[0/90/90/0]_2$ from 45 degree). Specimens were tested in tension, compression, shear, and fatigue.

2. Additionally, a Bostik adhesive was selected for bonding wind turbine segments together based upon over 300 interlaminar shear tests performed on 4 different adhesives with 3 different adhesive layer thicknesses. A full fracture toughness database was developed for all 4 adhesives.

Publications in 2018:

- Murray, R. E., Penumadu, D., Cousins, D., Beach, R., Snowberg, D., Berry, D., ... & Stebner, A. (2019). Manufacturing and Flexural Characterization of Infusion-Reacted Thermoplastic Wind Turbine Blade Subcomponents. *Applied Composite Materials*, 1-17.
- Cousins, D.S., Suzuki, Y., Murray, R.E., Samaniuk, J.R., Stebner, A.P. "Recycling Glass Fiber Thermoplastic Composites from Wind Turbine Blades," 2019, *Journal of Cleaner Production*, 209:1252–1263, 10.1016/j.jclepro.2018.10.286.
- Suzuki Y, Cousins DS, Dorgan JR, Stebner AP, Kappes BB. Dual-energy X-ray computed tomography for void detection in fiber-reinforced composites. Journal of Composite Materials. 2019 Jan 31:0021998319827091.

- Suzuki, Y., Cousins, D.S., Shinagawa, Y., Bell, R.T., Matsumoto, A., Stebner, A.P. "Phase Separation During Bulk Polymerization of Methyl Methacrylate," 2018, *Polymer Journal*, 10.1038/s41428-018-0142-7.
- Suzuki, Y., Cousins, D., Wassgren, J., Kappes, B.B., Dorgan, J., Stebner, A.P."Kinetics and Temperature Evolution during the Bulk Polymerization of Methyl Methacrylate for Vacuum-Assisted Resin Transfer Molding," 2018, *Composites Part A: Applied Science and*Manufacturing, 104:60–67, 10.1016/j.compositesa.2017.10.022.

Education and Outreach - Partial CHECRA Support

In 2018, the ICAMI project at the school of mines helped support one post-doctoral research associate, two Ph.D. graduate students, three hourly undergraduate students, and two summer undergraduate interns. Workforce development is a cornerstone of the ICAMI mission and the matching funds from CHECRA are critical in this aim.

Summary of benefits to the State of Colorado

- Support of the aforementioned research associates and students who will be highly desirable candidates for Colorado's rapidly growing workforce in the wind energy sector
- Large-scale investment by cost matching from industrial IACMI partners to universities in the state of Colorado
- Exposure of Colorado's intellectual and industrial resources in wind technology to a vast array of industry partners in the IACMI consortia
- Development of the state of the art CoMET facility at the National Wind Technology Center for wind turbine blade research and fabrication
- Ability for local industry and companies to use the School if Mines' extensive background in polymer science and state of the art facilities for mechanical testing

Engineering Research Center Reinvention of the Nation's Urban Water Infrastructure (ReNUWIt)
Colorado School of Mines
CHECRA Grant: $400,000 (per year for 10 years, renewed)
Reporting Period: January 1 - December 31, 2018

Summary: The Engineering Research Center (ERC) for Reinventing the Nation's Urban Water Infrastructure (ReNUWIt) at the Colorado School of Mines, under the leadership of Dr. John E. McCray, is a collaborative effort among four research universities: CSM, Stanford University, University of California at Berkeley, and New Mexico State University. The ERC was established on August 1, 2011 and is the first center to focus on civil infrastructure ever funded by the National Science Foundation.

Cities are facing a mounting water crisis from population expansion, ecosystem demands, climate change, and deteriorating infrastructure that threatens economic development, social welfare, and environmental sustainability. ReNUWIt's vision is to facilitate the transition of existing water supply systems, urban flood control, and wastewater treatment to a new state that will enhance the security and economic vitality of the nation's cities. Accordingly, the goal of this ERC is to advance new strategies for water/wastewater treatment and distribution, develop modular technologies and concepts, and prepare students to lead efforts to reinvent urban water infrastructure.

Description of the project, the principal persons or entities involved in the project, and the amount of funding allocated to each principal person or entity

To meet the challenges of reinventing urban water infrastructure, ReNUWIt has three research thrust areas defined as follows:
(1) **Urban Systems Integration and Institutions:** Support the reinvention and restoration of urban water systems through the development of decision-making tools that enable sound decision making about future investments in urban water infrastructure;
(2) **Efficient Engineered Water Systems:** Develop new, modular technologies to overcome barriers that prevent wider application of existing by underutilized technologies and collecting data on technical performance;
(3) **Natural Water Infrastructure Systems:** Develop technologies for managing natural systems to treat and store water while simultaneously improving urban aesthetics, with focus areas in stormwater treatment for beneficial use and groundwater recharge.

Water resource planners are hesitant to integrate new types of engineered treatment systems into their water portfolio due to uncertainties about cost, reliability, public health risks, and overall impacts on system performance. Thus, a mechanism for technology assessment is needed at scales ranging from the laboratory to the full-scale service area. Such capabilities do not exist and as a result, many good ideas are not brought into practice. To facilitate the integration of new technologies into urban water systems, tools like life-cycle assessment for decision-making are being advanced as well as conducting research and implementation of engineered systems. The strategic research plan continues to evolve in response to research outcomes, supplemental funding opportunities, and new information related to achieving ReNUWIt's overarching goals.

Within the *Urban Systems Integration and Institutions* thrust, research focuses on the development of integrated regional water models. The goals of the thrust area are to: (i) develop integrated decision support systems for utility planning; (ii) develop integrated visioning, assessment, and implementation tools for regional and municipal water planning; and (iii) identifying "technology diffusion pathways" to increase the likelihood of technology implementation. Mines is examining the legal, economic and technical feasibility of beneficial use of stormwater in a redeveloping neighborhood in northwest Denver (Berkeley neighborhood) including a method to project increases in impervious areas and the subsequent impact to stormwater flows and quality.

The goal of the *Efficient Engineered Systems* research thrust is to characterize the viability of existing but underutilized technologies at different scales by assessing their economic, environmental, and social costs and benefits. The specific aims of this thrust are: (i) develop improvements to energy and resource recovery from existing municipal wastewater systems; (ii) develop or asses new processes, approaches, and practices that support direct potable reuse of municipal wastewater; and (iii) advance (i) and (ii) to pilot-scale and full-scale demonstration and adoption. Research at Mines has incorporated smart system controls to monitor/ model/ optimize the hybrid sequencing batch-membrane bioreactor (SB-MBR) system operation for nutrient management (e.g., tailored water management).

The thrust area on the use of *Natural Water Infrastructure Systems* brings a much-needed quantitative approach to an area that has not previously been subjected to rigorous engineering analysis. The realigned goals of the thrust area are to: (i) develop novel approaches for manipulating subsurface natural system unit processes to predictably enhance stormwater and treated wastewater qualities; (ii) identify new ways of designing and operating unit process to maximize water quality and flood protection while enhancing function and aesthetics; and (iii) deploying sensors and actuators for real-time control and management of processes. Research at Mines is advancing passive treatment of stormwater through bioinfiltration systems and the hyporheic zone in streams.

Within the ReNUWIt framework described above, twelve projects were funded in 2018:

- Feasibility for Beneficial Use of Stormwater in Denver (U2.5);
- Long-term Sustainability of Stormwater Technologies (U2.13), joint with Colorado State University;
- Predicting Urban Water Demand for Infill and Redevelopment in Denver (U2.15);
- Reclaiming Energy from Wastewater using Anaerboic Digestion (E2.4);
- Tailoring Water Reclamation for Specific Purposes (E2.9, formerly E1.1);
- Chemical valorization of Energy from Waste (E2.12);
- Phosphorus Recovery in Existing Wastewater Treatment Facility Infrastructure (E2.16);
- Alternative Potable Reuse Treatment Trains (E3.4);
- Smart Engineered Wetlands (N1.2);
- Stormwater Infrastructure for Water Quality (N3.3); and
- Engineering Streambeds for Water Quality Improvement (N3.4).

Principal Investigators	Funding from CHECRA
John McCray, CSM Principal Investigator	
Center Lead	$29,330
Project co-Lead, Feasibility of Beneficial Stormwater Use in Denver, U2.5	$63,825
Project Lead, Long-term Sustainability of Stormwater Technologies, U2.13	$25,510
Project Lead, Engineering Streambeds for Water Quality Improvement, N.3.4	$23,637
Tzahi Cath	
Project Lead, Tailoring Water Reclamation for Specific Purposes, E2.9	$29,648
Linda Figueroa	
Project Lead, Reclaiming Energy from Wastewater using Anaerboic Digestion, E2.4	$12,350
Project Lead, Novel Phosphorus Extraction/Recovery in WWTF, E2.16	$39,162
Christopher Higgins	
Project Lead, Stormwater Infrastructure for Water Quality, N3.3	$6,431
Terri Hogue	
Project co-Lead, Innovative Stormwater Management in Denver, U2.5	$63,825
Project Lead, Predicting Urban Water Demand in Denver, U2.15	$29,383
Jonathan Sharp	
Project Lead, Smart Engineered Wetlands, N1.2	$4,015
TOTAL SPENDING (Jan-Dec 2018)	***$327,116***

Within the ReNUWIt projects (2018), full or partial support was provided to:

- 10 Doctoral students
- 5 Master's of Science Thesis students
- 19 Hourly Undergraduate students
- 7 REUs ~ a 10 week summer program designed to provide research experience for undergraduates
- 3 Post Doctoral Fellow
- 4 Research Staff
- 9 Faculty ~ 1 Assistant Professor; 2 Associate Professors; and 6 Professors

The manner in which each principal person applied the CHECRA funding in connection with project results

John McCray, Professor: Discretionary center funding for supporting new research directions. In support of the Denver Beneficial Stormwater Use project (U2.5) CHECRA funding supported partial salary support for Dr. McCray, partial support for one post-doctoral researcher, tuition, stipend and nominal materials for one PhD student, three undergraduate students to assist with frameworks and technical research to overcome policy and legal barriers to allow stormwater beneficial use and one teaching faculty for data synthesis in development of engineering drawing at Willis Case Golf Course. This work lead to a separate research directive focused on the evaluation of the long-term feasibility and sustainability of stormwater technologies (U2.13). In support of U2.13, CHECRA funding supported tuition and stipend for one PhD student.

One PhD student and nominal materials supported field scale testing and implementation of engineered urban streambeds for water quality enhancement thru BEST (N3.4). As an outcome of this work, Dr. McCray secured a partnership with the City of Golden, to engineer streambeds in stormwater channels to improve water quality. Mines and Golden jointly received a Proof of

Concept (POC) Innovation grant, awarded by an external technical advisory board of Colorado business entrepreneurs.

Tzahi Cath, Associate Professor: Funding for one PhD student focused on SB-MBR energy optimization and tailored non-potable reuse of treated wastewater (E1.1). This research is leveraged with a PhD student and materials supported by NSF funds.

Linda Figueroa, Professor: Funding provided support for six undergraduate students to sample and analyze the pilot scale anaerobic bioreactor at Plum Creek Wastewater Authority (E2.4) and partial salary for Dr. Figueroa for research oversight. Outcomes from this work have transformational changed in the current wastewater treatment paradigm. In addition, CHECRA funds supported tuition for two graduate students and hourly support for a undergraduate student working on phosphorus recovery within existing wastewater treatment facility infrastructure (E2.16). Both graduate students are currently employed with Metro Wastewater Reclamation District and are expected to directly implement research findings at the District.

Christopher Higgins, Associate Professor: Partial salary support for Dr. Higgins for his leadership role as N-Thrust Leader. In addition, one undergraduate student supported work with the City of Denver to develop of a field site at Cuernavaca Park and with the City of Golden for pilot scale testing of BioCHARGE (N3.3). This research is leveraged with a post-doctoral researcher, PhD student and materials supported by NSF funds.

Terri Hogue, Professor: One PhD student was partially supported for hydrologic modeling of the Berkeley neighborhood in northwest Denver and partial salary support for Dr. Hogue for student oversight (U2.5). Tuition and stipend for one PhD student is also provided focused on improving the understanding of factors affecting urban water use and projecting changes to water demand in Denver (U2.15). The broad goals of both of these efforts are to evaluate the potential for additional stormwater runoff generated due to increased infill development, develop high-resolution remote sensing methodologies for water use, and evaluating future stormwater scenarios based on infill and water demand. Nominal funds (<$500) were provided for expendable materials and supplies.

Jonathan Sharp, Associate Professor: Partial faculty salary support was provided for Dr. Sharp for his leadership roll as the Diversity and Inclusion co-Director for ReNUWIt across all partner institutions.

Results Achieved

Results from the *Urban Systems Integration and Institutions* thrust continued to focus on stormwater planning, management and treatment. In partnership with the City and County of Denver (U2.5), the technical, legal, policy and social barriers are being evaluated to enable beneficial use of stormwater runoff in the rapidly re-developing Berkeley neighborhood of west Denver. Modeling and stormwater quality sampling is being conducted for Denver to inform proposed new regulations for infill redevelopment in the City. For the State of Colorado, we are working with the Colorado Water Conservation Board (CWCB) and the State Engineer's office (SEO) to develop new policy to enable increased stormwater runoff from infill development to be utilized for beneficial use. Mines received a $50,000 grant from the National Science Foundation (NSF) to provide an internship for PhD student Ryan Gilliom with the CWCB and Colorado SEO to work on innovative policy to enable stormwater beneficial use. In addition, Professor McCray received a $60,000 grant from NSF to fund stakeholder workshops in the front range to brainstorm overcoming barriers to implementing beneficial stormwater use in the Front Range.

Results from the *Efficient Engineered Systems* research thrust continued to rely on field research on the Mines campus utilizing sequencing batch membrane bioreactor treatment of wastewater from housing at Mines (~7,000 gal/day), as well as pilot scale projects at two utilities in the Front Range (described in more detail below). The demonstration-scale treatment unit at Mines Park allows effluent qualities to be tailored to various reuse applications (i.e., urban landscape irrigation; streamflow augmentation; groundwater recharge) and continues to be supported through collaborations with manufacturers and start-up companies within Colorado. Identifying mechanisms (E2.9) by which nutrient removal can efficiently be achieved while lowering energy consumption is beneficial both from an energy resource standpoint and an economic perspective. Alternatively, E2.9 also investigates strategies for optimization of generating on-demand effluent qualities with elevated levels of nitrogen while simultaneously optimizing energy demands continue.

Demonstration scale Coupled Hybrid Anaerobic Reactors for Generation of Energy (CHARGE) have been operating at the Plume Creek Water Reclamation Authority (PCWRA) in Castle Rock for six years to evaluate the long-term viability of generating energy from wastewater. The project involves operations considerations such that small utilities can make use of an anaerobic treatment process to generate methane that can be used for energy while eliminating the need for aeration. The results from primary anaerobic treatment have led to additional investment by NSF ($329K; Sept 2015 – Aug 2018) and Water Environment Research Foundation (106K; May 2016 – Apr 2019).

A project to evaluate phosphorus extraction/recovery schemes and pilot scale implementation within existing wastewater treatment facility infrastructure was started in 2017 (E2.16). This project is part of an overall goal to recover valuable resources of energy and nutrients from wastewater. Metro Wastewater Reclamation District (District) is currently undergoing extensive upgrades to the Robert W. Hite Facility (RWHTF) to meet increasingly stringent nutrient regulations, particularly focused on effluent discharge phosphorus concentrations. Enhanced biological phosphorus removal (EBPR) is a sustainable and cost effective means to remove phosphorus from the liquid stream, however the process has been shown to negatively impact other process areas in both performance and cost. As a result, the District has continued developing near-term and potential long-term phosphorus management options, harnessing the experience of industry leaders and university expertise to make informed infrastructure and operating strategy decisions that best serve the 1.8 million Denver Metro area ratepayers. This project research will evaluate EBPR for improvements and optimization to maintain low effluent phosphorus concentrations while improving the effectiveness and efficiency of the RWHTF in other areas.

Results from the *Natural Water Infrastructure Systems* thrust continued to focus on developing smarter, more efficient methods for infiltrating recycled water for aquifer storage while simultaneously improving water quality. These sustainable technologies capitalize on the management of natural treatment processes to facilitate water treatment while enhancing storage infrastructure. For example, upscaling for field testing at the field scale of modules termed "Biohydrochemical Stream Water Treatment (BEST)" continued (N3.4). The BEST system was employed at a site by the City of Golden to mitigate stormwater runoff pollution. We are working with Golden to develop a second site. Mines received funding from the State of Colorado Innovation program to work with Golden. To our knowledge, this was the first grant given to an environmental-water project. A geomedia stormwater infiltration system

(BioCHARGE) was installed by the City of Denver at Cuernavaca Park for removal of dry-weather urban drool pollutants (N3.3). An outcome from this work was the successful DoD SERDP award ($491K; 2018 - 2020) to improve BMP stormwater treatment designs to prevent sediment recontamination.

Summary of Benefits to the State of Colorado

- Received $757,292 NSF core funds in 2018. These funds in combination with CHECRA funds ($400,000) and $178,586 CSM matching funds have supported:
    - 41 graduate students (tuition and stipend) in the first 7.5 years of ReNUWIt (2011-2017) with degrees in Civil & Environmental Engineering, Hydrologic Science and Engineering. Women comprised ~40% of these graduate students. Three existing graduate students are employed by either Metro Wastewater Reclamation District or the City of Denver.
    - Research experiences for 43 Mines undergraduates with ~50% of these students female.
- Continued collaboration with the City and County of Denver, the Urban Drainage and Flood Control District (UDFCD) to predict changes in stormwater management due to urban infill and development. A new collaboration with Southeast Metro Stormwater Authority (SEMSWA) was begun in October. We expect this partnership to result in collaborations with other stormwater management utilities in the Front Range.
- Collaboration with Metro Wastewater Reclamation District and Carollo Engineers investigating potential energy savings and treatment efficiencies associated with alterations in treatment plant operation for nutrient removal.
- A biohydrochemical enhancements for streamwater treatment (aka, BEST) pilot channel has been constructed with support from the City of Golden as well as from the State of Colorado Innovation Fund through a competitive grant process. In addition, Seattle Public Utilities provided $50k for installation recommendations for BEST stream restoration and floodplain reconnection tentatively planned for 2019.
- Successful pilot scale testing of anaerobic treatment process to generate energy at the Plum Creek Water Reclamation Authority has led to plans for expanding piloting at Littleton Englewood WWTP.
- Continued success obtaining new research grants at Mines to broaden the design and implementation of ReNUWIt developed treatment systems and approaches. These grants will support graduate and undergraduate students, many of which are expected to enter or remain in the Colorado workforce.
- Bi-monthly seminars organized and sponsored by the ReNUWIt students. Seminar speakers and topics include a range of student research, industry partners, and experts.
- A new collaboration between ReNUWIt at Mines and the Urban Water Innovation Network (UWIN), an NSF Sustainability Research Network (SRN) at Colorado State University was established. A student and faculty member at Mines are working with a student and two faculty members at CSU to evaluate sustainability of ReNUWIt water green infrastructure (GI) technologies compared to traditional GI technologies.
- ReNUWIt gave numerous workshops. "lunch and learns", and technical outreach talks to stakeholders in the Front Range, including the Colorado Stormwater and Floodplain Managers Association (CASFM), Wright Water Engineers, Southeast Metro Stormwater Authority (SEMSWA), Denver Water, and City and County of Denver.
- Numerous front range water professionals came to Mines to give talks and workshop at the invitation of ReNUWIt, particularly in the Environmental Engineering Seminar Series and the ReNUWIt student group (SUWIR) seminar series.

- Students and faculty remain very active with outreach efforts:
  - Third summer of the 6 week NSF Research Experience for Teachers (RET) Summer Program (PI Hogue) bringing K-12 teachers from Jefferson County and Denver Public Schools to the Mines campus
  - Project-based water filtration learning: three classroom sessions of five 1.5-hour sections in Lakewood High School's Conceptual Chemistry class designing and building prototype filters to address water quality issues in Australia, Canada, Kenya, and India
  - Webinar (C. Bellona) for the American Waterworks Association (AWWA) on Focusing on the brine: Membrane research on resource recovery, and emerging contaminants
  - Hosted high school students conduction water treatment exercises for the Society of Women Engineers, Girls Lead the Way Program, Golden, CO
  - Elementary Math & Science Night at Mitchell Elementary, Golden, CO and Shelton Elementary, Golden, CO
  - Water treatment introduction to 3rd graders at Schaefer Elementary
  - Denver Metro Water Festival, Denver, CO
  - Reoccurring tours at the Mines Park test site and interaction with Girls in STEM, Lakewood, CO
  - Numerous presentations to underrepresented professional organizations on campus (i.e., Society of Black Engineers, American Indian Science and Engineering Society, Society of Asian Scientists and Engineers)

Publications in 2018 (funded wholly or in part with CHECRA funds):

<u>Thesis and Dissertations:</u>

Erikson, Rebecca (2018). Stoichiometry and Kinetics of the Microbial Degradation of Substrate in an Anaerobic Baffled Reactor. M.S. Thesis. Civil and Environmental Engineering, Colorado School of Mines, Golden, CO.

Li, Yalin (2018). Valorization of Wastewater-Derived Biomass via Integrated Aqueous Systems. PhD. Dissertation. Civil and Environmental Engineering, Colorado School of Mines, Golden, CO.

Vatankhah, Hooman (2018). The Role of Ozonation in Potable Reuse Treatment Trains. PhD. Dissertation. Civil and Environmental Engineering, Colorado School of Mines, Golden, CO.

<u>Publications, Presentations, and Posters</u>

Burant, A, W Selbig, E Furlong, C Higgins (2018). Trace organic contaminants in urban runoff: Associations with urban land use. *Environmental Pollution*, 242: 2068-2077. DOI: 10.1016/j.envpol.2018.06.066

Cherry, L, D Mollendor, W Eisenstein, T Hogue, K Peterman, J McCray (2019). Predicting parcel-scale redevelopment within the Berkeley Neighborhood in Denver Colorado using linear and logistic regression, submitted to *Sustainability J.*

Coffey, C, A Pfluger, J Munakata Marr L Figueroa (2018). Treating anaerobic effluents: nitrogen removal from mainstream anaerobic wastewater treatment using partial nitration and anammox. RMSAWWA/RMWEA Joint Annual Conference, September 2018, Denver, CO.

Gilliom, R, C Bell, T Hogue, J McCray (2018). Improving parameterization of green infrastructure pollutant removal rates utilizing the international stormwater BMP database. AWRA Annual Conference, November 2018, Baltimore, MD.

Gilliom, R, A Kroepsch, T Hogue, J McCray (2018). Using policy and historic conflict to inform research agenda: Infill development and stormwater harvesting. Presentation at AWRA Annual Conference, November 2018, Baltimore, MD.

Herzog, S, C Higgins, K Singha, J McCray (2018). Performance of engineered streambeds for inducing hyporheic transient storage and attenuation of resazurin. *Environ. Sci. & Technol.*, 52(18): 10627-10636. DOI: 10.1021/acs.est.8b01145

Herzog, S, K Peter, Z Tian, C Wu, J McCray, K Lynch, E Kolodziej (2018). Quantifying attenuation of hundreds of organic stormwater contaminants by a restored urban hyporheic zone, Geol. Soc. Amer., Abstracts with Programs. 50(6), DOI: 10.1130/abs/2018AM-319585

Higgins, C, S Herzog, B Halpin, A Portmann, N Fitzgerald, W Eisenstein, J McCray (2018). Hyporheic zone management through biohydrochemically enhanced streamwater treatment (BEST) modules. Poster, Gordon Research Conference, June 2018, Plymouth, NH.

Jones, Z, K Mikkelson, M Nygren, D Sedlak, J Sharp (2018). Establishment and convergence of the photosynthetic microbial biomats in shallow unit process open-water wetlands, *Water Research*, 133: 132-141.

Lee, U, C Criddle, M Geza, T Cath, D Freyberg (2018). Decision support toolkit for integrated analysis and design of reclaimed water infrastructure, *Water Research*, 134(2018): 234-252.

Leow, S, B Shoener, Y Li, J DeBellis, J Markham, R Davis, L Laurens, P Pienkos, S Cook, T Strathmann, J Guest (2018). A unified modeling framework to advance biofuel production from microalgae, *Environ. Sci. & Technol.*. 52: 13591-13599. DOI:10.1021/acs.est.8b03663

Li, Y, W Tarpeh, K Nelson, T Strathmann (2018). Quantitative evaluation of an integrated system for valorization of wastewater algae as bio-oil, fuel gas, and fertilizer products. *Environ. Sci. & Technol.*, 52: 12717-12727. DOI: 10.1021/acs.est.8b04035

McCray, J (2018). Engineered streambeds for water quality enhancement in urban streams, Developments in Irish Hydrogeology in a Changing Water Services and Planning Environment, Keynote Address 38th Annual Groundwater Conference, International Association of Hydrogeologists – Irish Group, Tullamore, Co. Offaly, Ireland, April 2018.

McCray, J, K Gustafason, K Slinski (2018). Urban stormwater-quality sampling program: Under the streets, or.... data driven decision making – Is it better, Presentation, Colorado Stormwater Council, October 2018.

McCray, J, K Gustafason, K Slinski, R Gilliom, J McGovern, T Hogue (2018). Stormwater quality related to infill development in Denver: Results of storm sewer monitoring, Geological Society of America Abstracts with Programs. 50(6), DOI: 10.1130/abs/2018AM-323669

Munakata Marr, J (2018). Genetic analysis of wastewater microbial communities. Presentation, Rocky Mountain Water Environment Association Vail Professional Wastewater Operators Meeting, October 2018, Vail, CO.

Odom, G, K Newhart, T Cath, A Hering (2018). Multi-state multivariate statistical process control, *Applied Stochastic Models in Business and Industry*, 1-13.

Panos, C, T Hogue, R Gilliom, J McCray (2018). High-resolution modeling of infill development impact on stormwater dynamics in Denver, Colorado. *J. Sustainable Water in the Built Environ*, DOI: 10.1061/JSWBAY.0000863

Panos, C, T Hogue (2018). Evaluating urban resilience to hydrologic change by modeling future impervious cover change due to infill development. Presentation, 9th International Congress on Environmental Modeling and Software, Fort Collins, CO.

Panos, C, T Hogue, J McCray (2018). Modeling and management of urban stormwater runoff in a neighborhood of Denver, CO. Poster, American Geophysical Union (AGU) Fall Meeting, Washington DC.

Pfluger A, J Callahan, J Stokes, D Ramey, L Figueroa, J Munakata Marr (2018). Energy positive wastewater treatment: Life-cycle analysis of mainstream anaerobic treatment of domestic wastewater, *Environ. Sci. & Technol.*, 52(18): 10500-10510.

Pfluger A, J Starke, S Cosper, J Munakata Marr, L Figueroa (2018). Biogas generation from waste: Overcoming barriers to widespread implementation of anaerobic technologies in DoD for energy security, *The Military Engineer.*

Pfluger, A, R Erickson, G Vanzin, M Hahn, J Munakata-Marr, L Figueroa (2018). Energy-generating potential of biologically enhanced anaerobic primary treatment of domestic wastewater using multiple-compartment bioreactors, *Environmental Science: Water Research & Technology*, 4:1851-1866. DOI: 10.1039/C8EW00237A

Pfluger, A, M Hahn, A Hering, J Munakata-Marr, L Figueroa (2018). Statistical exposé of a multiple-compartment anaerobic reactor treating domestic wastewater, *Water Environment Research*, 90: 530-542. DOI: 10.2175/106143017X15131012153068.

Pfluger, A, G Vanzin, J Munakata Marr, L Figueroa (2018). Succession of a founding microbiome after seeding in a multiple-compartment anaerobic bioreactor for domestic wastewater treatment. Poster, Rocky Mountain GeoBiology Symposium, April 2018, Golden, CO.

Pfluger, A, G Vanzin, R Erickson, C Coffey, J Munakata Marr, L Figueroa (2018). Coupled primary and secondary anaerobic treatment of domestic wastewater for energy generation: biochemical reactor construction, operation, and modeling. Poster, National Renewable Energy Laboratory – Mines Joint Bio Workshop, January 2018, Golden, CO.

Tarpeh, W, J Barazesh, T Cath, K Nelson (2018). Electrochemical stripping to recover nitrogen from source-separated urine, *Environ. Sci. & Technol.*, 52(3): 1453-1460

Vanzin, G, A Pfluger, J Munakata Marr, L Figueroa (2018). Metagenomic analysis of an energy-positive anaerobic hybrid reactor system for treatment of domestic wastewater under psychrophilic conditions. Poster, Rocky Mountain GeoBiology Symposium, April 2018, Golden, CO.

Vatankhah, H, C Murray, J Brannum, J Vanneste, C Bellona (2018). Effect of pre-ozonation on nanofiltration membrane fouling during water reuse applications, *Separation and Purification Technology*, 205(31): 203-211.

Warsinger, D, S Chakraborty, E Tow, M Plumlee, C Bellona, S Loutatidou, L Karimi, A Mikelonis, A Achilli, A Ghassemi, L Padhye, S Snyder, S Curcio, C Vecitis, H Arafat, J Lienhard (2018). A review of polymeric membranes and processes for potable water reuse. *Progress in Polymer Science* 81: 209-237.

TOF-SIMS 2019 MRI Update

(a) A description of the project, the principal persons or entities involved in the project, and the amount of funding allocated to each principal person or entity;

The project consisted of the acquisition of a Time-of-Flight Secondary Ion Mass Spectrometer (TOF-SIMS), a highly unique instrument capable of measuring and mapping chemical species at low concentrations in solid samples. The instrument is open for use on a cost-recovery basis to all academic entities in the state, and at an industrial rate to companies. CHECRA funds were used as partial required cost share in a competitive National Science Foundation (NSF) competition. CHECRA funds in the amount of $216,759 were used for supporting instrument acquisition (84%) and partial staffing of the instrument in the first few months (16%). Funds in the amount of $999,600 were awarded by NSF and used towards instrument acquisition.

Principle Persons:

PI/PD - Corinne E Packard, PhD (cpackard@mines.edu) -no funding support
CO-PI/PD - Corby G Anderson, PhD (cganders@mines.edu) - no funding support
CO-PI/PD - Melissa D Krebs, PhD (mdkrebs@mines.edu) - no funding support
CO-PI/PD - Angus A Rocket, PhD (arockett@mines.edu) - no funding support
Research Specialist- Michael Walker- (mawalker@mines.edu) - $35,715 total ($26,416 salary + $9299 fringe)

(b) The manner in which each principal person or entity applied the funding in connection with the project; and

The TOF-SIMS instrument completed installation Aug 3rd, 2018 and was immediately put to use that day to support research conducted by a post-grad student in the field of ceramics. Research Specialist, Michael Walker, was hired to support the instrument. He began work on the day of the instrument installation and is primarily responsible for machine maintenance and calibration, equipment operation and data analysis, student training, instrument scheduling and billing, marketing of capabilities, and industrial outreach. Currently the TOF-SIMS project does not receive faculty funding support; following expenditure of the CHECRA funds, we have transitioned to being fully supported by cost recovery recharge.

(c) The results achieved by the project.

Since Sept, 2018 usage on the instrument has averaged over 20hrs/week in direct billing, which includes data acquisition, data analysis, and reporting of TOF-SIMS data in support of research across many fields of study: ceramics, solar power, steel manufacturing, medical instruments, and catalysts in fuel cells.

The TOF-SIMS has also been used to assist other Universities in their individual research projects, either through already established research collaborations with Mines, or through new established research projects with Colorado State University, the University of Illinois Chicago, the University of Sothern Florida, the University of Denver, and Old Dominion University.

This project has already established a working relationship with a local steel manufacturing company, providing them with crucial data to identify chemical defects in their manufacturing process. Additional industrial relationships are being developed with a battery cell manufacturer and an electronic components manufacturer.

Additionally, the instrument has been used for educational outreach, by providing tours to K-12 students and teachers, and university classes in surface analysis and biomedical engineering.

2018 Annual Report for CHECRA matching funds for McKay ARPA-E project

Root genetics in the field to understand drought adaptation and carbon sequestration – PI, Professor John McKay, CSU

ARPA-E ROOTS Award
Colorado State University
CHECRA Grant ($325.6K over 3 years)

Summary: We are working to develop a high-throughput phenotyping platform to measure root system traits, soil carbon and nutrients, as well as mapping soil surface greenhouse gases (GHG). This platform will be used in field experiments to identify genetic variation in root traits and their effect on soil C stocks and GHG. This understanding will then be used to improve root trait-based model predictions of soil GHG emissions and soil carbon sequestration to depth in an integrated project advancing both trait development and field screening. The project started on 3 July 2017.

Description of the project, the principal persons and the amount of funding:
We will utilize a diverse set of maize lines to examine for root structure and composition under full and limited irrigation in Colorado and Arizona. They will be phenotyped with our existing approaches as well as newly developed root (root pulling force) and soil HTP approaches. The understanding derived from these experiments and the data on root and soil response variables will be used to develop and evaluate a new generation process-based model, to be used to enhance translation and improve throughput of breeding as well as a tool to quantify the impacts of root parameters across ideotypes on soil C sequestration and GHG emissions in different environments. For category 2 we will develop novel sensors, incorporating them into our already functioning field HTP systems. The most promising methods and sensors will be used to identify genomic regions that influence root and soil traits and their sensitivity to drought by screening large mapping populations in the field. Data from this larger field effort will be used to validate the new model. The principal persons involved at Colorado State University are PI John McKay, as well as Co-PIs Francesca Cortufo, Greg Graff, Sangmi Pallickara and Keith Paustian. ARPA-E officials made the decision to terminate task 4, led by Co-PIs Randy Bartels and Thomas Borch, after the task failed to meet milestones.

Funding from CHECRA and allocation:
The CHECRA funds have been used to support PI John McKay, Research Scientist Jack Mullen, and project manager Anne Howard. The CHECRA funds have also enabled purchase of an EarthSense TerraSentia high-throughput phenotyping robot to enhance our field measurement capabilities.

Results Achieved:
Technology to Market

We have finalized our advisory board and involved them in our annual team meetings in November 2017 and 2018. Members of the advisory board include the following:

- Dr. Rene Lafitte, Research Fellow, Pioneer DuPont
- Dr. Stephen Wood, Soil Scientist, Global Lands Team, The Nature Conservancy
- Matthew Powell, Founder, Chief Science Officer, AgWorld
- Dr. David Brown, Director of Engineering, PivotBio
- Dr. Damian Allen, Platform Leader, Shell

Ongoing discussions with our advisory board and other potential customers/partners have allowed us to develop and update a value model for this project (Figure 1). We are exploring interest of investors in agtech more broadly, as well as a couple of the

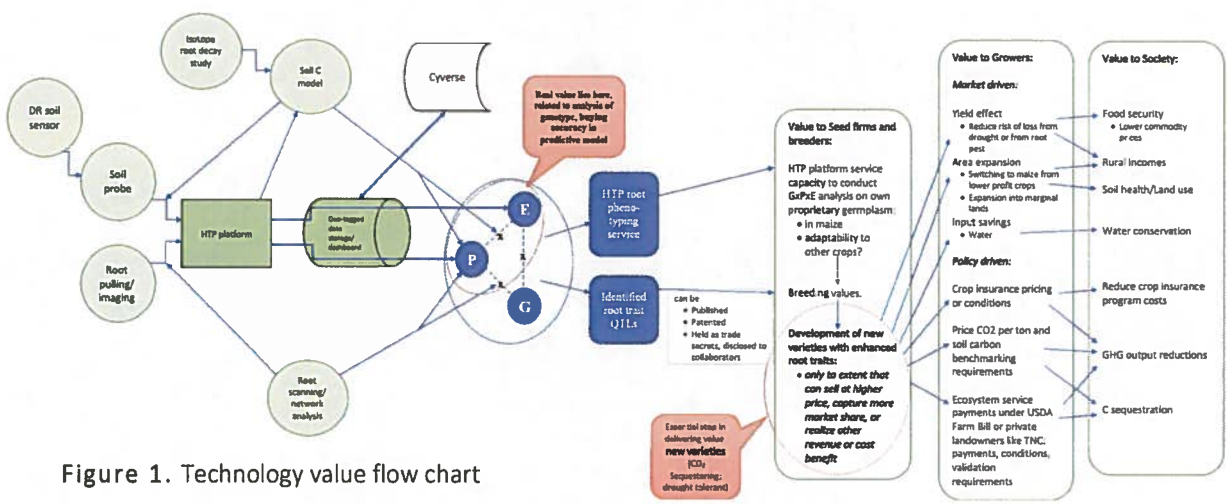

Figure 1. Technology value flow chart

candidate technologies being developed under this project.

We are inquiring about growers' commercial interest in enhanced root varieties. Colorado Corn has assisted us in recruiting about a dozen corn growers for in depth interviews. We have developed a qualitative questionnaire and our process is underway to conduct interviews throughout 2019 to inform our value model. We will also be developing an economic model of farmer adoption incentives of maize with enhanced root traits.

We met with experts from the USDA Economic Research Service on adoption of drought tolerant corn varieties in the United States. They are in the process of releasing a new study based upon Agricultural Resource Management Survey (ARMS) data of field level adoption of drought tolerant varieties. This data provides a key indicator of potential commercial interest in enhanced root corn varieties.

We have held preliminary discussions with a representative from the Brazilian Sugarcane Ethanol Association about the status of high-throughput phenotyping in sugarcane breeding programs at Centro de Technologia Canavieira (CTC) (the Sugarcane Research Center) and startup companies located in the associated Piracicaba Technology Park in Piracicaba, Brazil. There may be interest in adapting methods developed for maize to sugarcane. Root mass of this semi-perennial monocot could be a significant carbon sink.

Development of RPF and CSS instruments

We have worked with the Colorado-based engineering company Czero to develop two novel systems—a Root Pulling Force (RPF) sensor and a Crop Soil Sampling (CSS) system with a design that supports both systems on a common structural frame. For current work on the control systems, Czero broke the design down into three subsystems and one master controller to oversee the other three.

1. RPF sensor – The main objective of the RPF sensor is to collect root pulling force data for individual maize plants. The controller for this subsystem must identify a plant and position the gripper in the proper location to execute a pull. After a plant is pulled, the controller moves the plant to a location to remove dirt from the root ball and photograph the root structure. The control system must be able to tag each photo and correlate each set of pull data the extracted plant's location in the field. An invention disclosure for this system is in progress.

2. Crop Soil Sampling (CSS) system – The main objective of the CSS system is to extract and package soil samples from the various depths in the ground. The controller for this subsystem must control a hydraulic cylinder to take a soil core up to one meter deep and pull the core from the ground. The soil sampling system must take samples at various locations along the core and package those samples for later analysis. The control system must be able to tag each soil sample with the plant's location in the field and the depth of the sample. Czero designed a mechanism that could extract a column of soil from the ground up to one meter deep. The primary component of this mechanism was a long coring tube that was driven into the ground hydraulically, then pulled out to extract the core. The concept selected to perform this task uses .410 shotgun shells that are pushed horizontally through an opening in the coring tube which hangs vertically.

3. Linear Positioning System (LIPS) – In order to provide a stable platform for the RPF and CSS systems, a single frame containing the two systems is placed on the ground and held there during data collection. Because the tractor continues to move through the field as the data is collected, any relative motion between the two must be isolated. The main objective of the LIPS is to isolate movement between the combined system frame and the tractor during soil sampling. This is achieved through a combination of controlled hydraulic cylinders and linear actuators that work to keep the combined frame grounded throughout data collection. Detailed design of the linear positioning system, combined frame system, and the ground penetrating portion of the CSS is well under way. Once the structural components have been completed, integration of the root ball cleaner, photography station, plant identification sensor, etc. can occur.

The high clearance tractor, upon which the systems described above will be mounted, was delivered in early January 2019.

Field tests of the RPF system were performed on full grown maize plants. The stationary test stand was deployed in the test fields at ARDEC in Fort Collins, Colorado to perform pull tests. 50 test pulls were performed using a range of test parameters to determine the optimal pulling conditions for full grown plants. The parameters were pushed to the extremes in order to induce failed pulls so that optimal operating conditions could be identified. Preliminary data suggests that root biomass is strongly predicted by manual RPF (r^2 = 0.66, Figure 2).

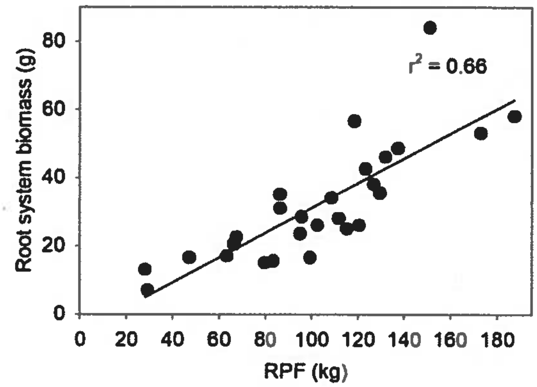

Figure 2. Correlation between RPF and root system biomass of maize lines

Field tests were also performed to test soil sampling from the coring tube. The primary purpose of these tests was to determine the forces required to drive the empty sample shell into an opening in the soil tube, and to observe what effect the sample tube opening size and shape had on the sample extraction. Soil cores were taken using an off the shelf coring tube. The extracted core was then transferred to a similarly sized PVC pipe that had various size and shape openings drilled into it. A drill press was used to drive the sample containers into the soil core to ensure straight perpendicular sampling.

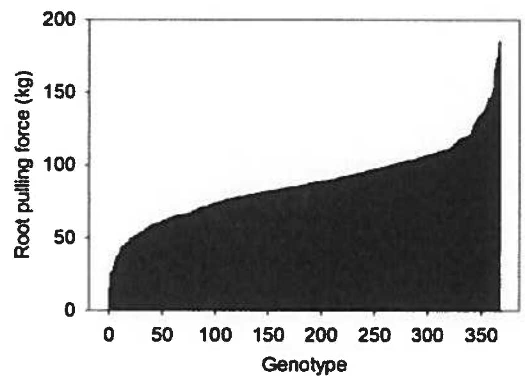

Figure 3. Average RPF for all genotypes under limited irrigation in September.

Field Experiments in Colorado and Arizona

361 genotypes were planted at Colorado State University's Agricultural Research, Development, and Education Center (ARDEC) in Fort Collins, Colorado. Four lines (NAM RILs) were selected for extreme root traits and are highly replicated. The remaining 357 lines are SAM inbred lines. We also grew a panel of maize genotypes for collaborators at Pennsylvania State University (PSU) under full and limited irrigation.

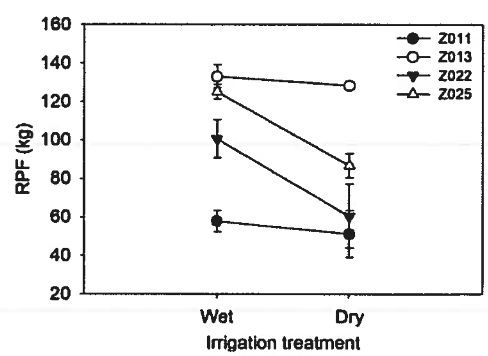

Figure 4. Average end-of-season RPF of four extreme maize lines under full and limited irrigation

We took root pulling force (RPF) measurements at two time points; the first in late July and the second in early September. At both time points we took measurements from the full diversity panel over all replications and treatments. This resulted in approximately 4000 root systems and their respective stalks over both time points, which are being processed for additional trait measurements. We also took regular flowering notes and one time point of leaf water content. Initial data analysis shows that there is a significant genotype effect on RPF (Figure 3). We grew four extreme lines, selected for varying root lignin content, in high replication with the rest of our maize lines this summer. Figure 4 shows the average root pulling force measurements between full and limited irrigation regimes for the four extreme lines, which exhibit differential sensitivity to drought.

2D images were taken of all root systems. Differences among genotypes in root system architecture (Figure 5) may improve predictions of root biomass and drought performance. We are working with the Danforth Plant Science Center for further 3D X-ray CT imaging of root systems. We have also sent a subset of roots for suberin analysis at the University of Nevada, Reno, and have sent the remainder of the roots from the September pulling to Ward Laboratories in Kearney, Nebraska for lignin composition analysis.

A subset of the same germplasm was grown under the same design at University of Arizona's Maricopa Agricultural Center (MAC). The same phenotypes described above were taken in Maricopa over several time points.

The EarthSense TerraSentia Robot was optimized throughout the field season and will continue to be used in the 2019 field season.

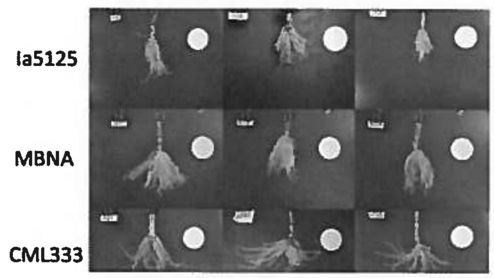

Figure 5. Examples of variation in root system architecture among lines.

Benefits that the project has brought to Colorado

The project continues to fund dozens undergraduate and graduate students as well as 8 post-doctoral researchers. Through our collaboration with PSU and our work under this project we are continuing to improve Colorado State University ARDEC's capabilities as a national drought research center. Our work on this project with Colorado corn farmers will contribute to our knowledge of incentives that will increase drought adaptive and root enhanced maize varieties.

MRI: Acquisition of a Maskless Lithography System

NSF-MRI Award # 1727044
PI Kristen Buchanan
Co-PIs Stuart Field and Mingzhong Wu
Department of Physics, Colorado State University
Project period: 09/15/2017 - 08/31/2020
CHECRA Grant ($66,482 over 3 years)
Date of report: February 18, 2019

Summary: This award is an instrumentation award that has enabled the acquisition of a maskless lithography system at Colorado State University (CSU). Photolithography is a critical capability for nanoscale and materials science and this award has allowed CSU to acquire a maskless lithography system that is enabling a wide range of nanoscience-related research at CSU and at neighboring institutions in the Northern Colorado/Wyoming area. The instrument has a high resolution, determined to be 0.6 microns upon installation, and the ability to easily align to pre-existing patterns. This tool is optimized for the direct writing of lithographic patterns over a small area and is well suited to a research environment where the ability to easily reimagine and redesign a sample is a particular asset. The new maskless lithography system is being used for a variety of research projects including studies of spin dynamics in magnetic nanostructures, superconducting vortices in films with micron-scale features, and novel spintronic devices. Other projects that will benefit from this new capability will use the tool to add electrical contacts to ZnO nanorods, to create novel micron-sized biosensors on silicon and glass, to fabricate nanostructures that have unique properties of wettability, and to make high-efficiency solar cells. The instrument is being operated as a user-accessible tool and is available to any interested users. It will enable new research and will be directly benefit students. Since there are more than 28 research groups in the northern Colorado/Wyoming region that have a need for this instrument we expect that our already robust user base will continue to grow.

Funding from CHECRA and allocation: The CHECRA funds have been used to support the mandatory cost share for an NSF-MRI proposal. The NSF provided $212,031 towards the purchase of a maskless lithography system; the CHECRA funds **($66,482)** were used in part towards the purchase of the instrument, and then the remainder is being used to support graduate students who are developing training materials and a web site to advertise the tool, maintaining the instrument, and training users.

Major Activities: Major activities carried out to date for this project include the acquisition and installation of the maskless lithography system, training of our first users, and the development of a web site and initial user access and training procedures. A committee to oversee the instrument user program has also been established that includes two of the PIs of this grant (Kristen Buchanan and Stuart Field), Justin Sambur (Chemistry), Tom Chen (Electrical and Computer Engineering). The committee is in place to set user fees and to handle any issues pertaining to maintenance or scheduling. The maskless lithography system that was acquired is the LW405C laser writer produced by Microtech s.r.l. of Italy. The system was installed in April 2018. In our proposal, 20 research groups were identified as potential users; at least 8 additional groups have been identified since then. A technician was hired for the summer of 2018 and developed training materials and a web site for the instrument. Student training has commenced, and the tool is already being used frequently for projects in nanomagnetism and spintronics, superconductivity, and drug uptake studies. The usage of the instrument has consistently been between 80 and 110% of business hours since it was opened up for general usage in April of 2018. The installation and training from the company included a training seminar on the instrument and this was attended by 45 people including 5 remote participants from Denver, Wyoming, Colorado School of Mines, and a local company, Broadcom. The advertisements of this system via the seminar announcements lead to the identification of 7 additional research groups whose research will benefit from this new capability, and some of these new groups have already scheduled training. We have since added a new faculty member from Colorado School of Mines to our list of interested users.

We hired a dedicated half-time technician, Gus DeMann, also a PhD student in the Physics department, for the summer to develop the web site and training materials for the instrument, and to train students on the instrument during what we anticipated to be one of the busiest training periods of the year. Gus has extensive photolithography experience and has been a valuable asset for training and growing the user base for the instrument. Thus far 32 users have been trained. Selected students and faculty were trained by Microtech during their installation/training visit and since then new users have been trained by Gus. During the academic year we have a half-time graduate researcher position to handle training and instrument maintenance and in the summer this will be a full time position since we anticipate higher demand for training during this time period, and we also plan to offer a short course workshop on photolithography during the summer. Gus also helped to develop a web site to advertise the instrument and host training materials:
http://physlabs.colostate.edu/lithography/
The web site includes information on the instrument capabilities, examples, and details on how to gain access to the instrument.

The instrument is already being used frequently for projects in nanomagnetism and spintronics, superconductivity, and drug uptake studies. Some examples of some of the work that has been done thus far are shown in Figures 1 and 2.

Fig. 1: Fiona McCluskey (left) and Tori Dang (right), undergraduate students from Bryn Mawr College who worked at CSU for Kristen Buchanan's group last summer, are patterning copper hoops for research on the effects of Dzyaloshinskii Moriya interactions (DMIs) on spin dynamics and on skyrmion formation. The samples will be characterized using micro-focus Brillouin light scattering. The image on the right shows a patterned hoop in S1813 on top of magnetic structures made by Tori and Fiona using the lithography system. The hoop inner diameter is 20 μm. The smaller circles are patterned multilayered magnetic structures that will be used to study the effects of DMI on spin dynamics.

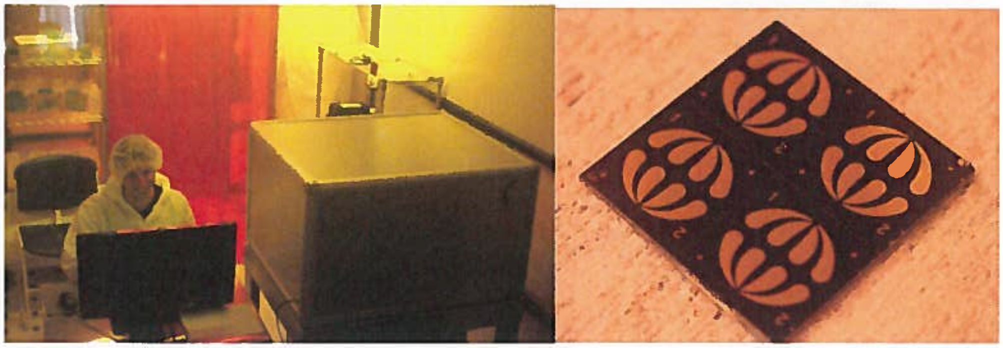

Fig. 2: Weston Maughan, a graduate student in Stuart Field's research group, writes an open relief area on a silicon wafer that will later be etched away. This is one of several steps required to create a superconducting nanowire. The image on the right shows an array of gold electrical contacts patterned on a 16 x 16 mm silicon wafer. These leads are being used for studies of superconducting vortices by the Field group.

Thus far 32 users have been trained, where the vast majority are students and the remainder are faculty and research associates/postdocs. Five of the students who have used the instrument are undergraduates, four of the undergraduate students are women, and three of the graduate students who have or will soon be trained are women. Almost all of the students, postdocs, and faculty who have used the system are from Colorado, with the exception of three of the undergraduate students who came to CSU from smaller institutions for summer research programs including an NSF-funded Research Experience for Undergraduate Program. The students are acquiring valuable photolithography skills that will translate well to future research endeavors in academia or in industry.

Benefits that the project has brought to Colorado: The CHECRA funds were used to support the purchase of the instrument and the salaries for graduate students who are training new users. The students are benefitting directly from the opportunity to improve their photolithography and teaching skills, and the instrument significantly enhances CSU's photolithography capabilities. The instrument is being used by students and researchers from three colleges at CSU and is attracting widespread interest from not just researchers at CSU but also from other institutions in Colorado and Wyoming. Many cutting-edge areas of research in physics, engineering, chemistry, and biology depend on the ability to make structures with sizes of a micron or less. This instrument is being used for research that is relevant to technology, especially solid-state electronics including magnetoelectronic (spintronics) devices, and biomedical research that are beneficial to society. Because the instrument has a user base with such broad interests, we anticipate that it will facilitate interactions between user groups and new cross-disciplinary scientific collaborations. It will also help to broaden interactions with local companies. One of the participants in the initial training seminar was from Broadcom's Fort Collins location, a company that has an active interest in micro and nanofabrication. A total of 28 research groups have been identified as potential users. Most are from Colorado State University from the Departments of Physics, Electrical Engineering, Chemistry, Biological Sciences, Chemical and Biological Engineering, and Mechanical Engineering. One is a local company (Broadcom). We also have users from Colorado School of Mines (M. Singh's group, and Serena Eley) and the University of Denver (B. Zink's group). Based on the large number of faculty and students who have expressed interest in this tool from CSU and the surrounding area, we anticipate that the user base we already have (32 trained users) will continue to grow. This instrument is being used to teach a broad range of undergraduate and graduate students and postdocs photolithography skills that will translate well to a variety of research areas in academia, government research labs, and industry. The PIs are also giving tours to student groups like the Society of Physics Students and using this as an opportunity for outreach to members of the local community.