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

March 1, 2017

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 Senators and Representatives:

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 2016.

The CHECRA was created to provide a source of matching funds for National Science Foundation (NSF) and other federal grants that require or benefit from a state match. CHECRA funding has helped to bring significant research dollars to Colorado. The following projects received CHECRA funding in 2015:

University of Colorado (CU)

- 1. In 2014, the NSF awarded the University of Colorado a 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 liquid crystal frontiers, an area where the University of Colorado is among the leading authorities, and work related to DNA nano-science. The CHECRA has pledged \$400,000 per year for six years; 2016 was the third 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; 2016 was the first year of funding.

Colorado State University (CSU)

- 3. The Accelerating Innovation Research Research Alliance (AIR-RA) project at CSU, funded by NSF, is advancing research in cadmium telluride photovoltaics with the vision of making PV electricity a major source of energy. The CHECRA made the second of three payments of \$132,000 toward this project.
- 4. DOE High Energy Physics Accelerator CSU received funding from the US Department of Energy for *Innovative solutions for scaling high energy femtosecond diode-pumped lasers to multi-kilowatt average power for compact accelerators and application*. CHECRA made a one-time payment of \$90,000 toward this project.

Colorado School of Mines

- 5. 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 who are partnering with the federal government to create a manufacturing hub focused on U.S. leadership in next-generation materials. 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 200,000 per year for five years, beginning in 2015. CHECRA made a single payment of \$100,000 in 2016 to the School of Mines.
- 6. A project at Colorado School of Mines called Water Quality and Supply Impacts from Climate-induced Insect Tree Mortality and Resource Management in the Rocky Mountain West received the fifth of five payments of \$75,000 in 2015. This five-year effort funded by NSF is studying water resource changes resulting from the mountain pine beetle epidemic.
- 7. The NSF renewed the Colorado School of Mines' Re-inventing the Nation's Urban Water Infrastructure (ReNEWIt) Engineering Research Center, for which CHECRA agreed to provide a continued cost share of \$400,000 per year for five years. CHECRA made the first of five payments in 2016. 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.
- 8. The CHECRA provided cost shares for two Major Research Instrumentation (MRI) grants from NSF in 2015. These grants provide higher education institutions with major instrumentation that supports the research and research training goals of the institution and that is also used by other researchers regionally or nationally. The CHECRA Board determined that these grants play a significant role in encouraging collaboration among institutions in Colorado and beyond in areas of common research interest that positions researchers to compete for additional federal research grants. Following are the awards and amounts CHECRA provided:

University of Colorado: Acquisition of an Inductively Coupled Plasma Dry Etching System for Highly Controlled Etching of Chalcogenides and Related Compounds; \$143,558. This equipment will be made available to local industry and other institutions;

students will learn new skills and thus be better prepared for jobs in leading-edge industries; the lab also hosts visits by K-12 students.

Colorado School of Mines: Environmental X-ray Photoelectron Spectroscopy Facility -- \$247,050.

Attachments 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 have many additional positive benefits to 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.

Some highlights of these benefits to Colorado include:

- The University of Colorado's Materials Research Science and Engineering Center has a K-12 outreach program that in just the last year held 130 classes, reaching 3,500 K-12 students with physical sciences presentations that fit the curriculum at schools. The Center has a specific partnership with Arrupe High School, an urban high school that serves economically disadvantaged families, under which it introduced high schools students to such concepts as polymers and DNA extraction.
- CU's MRSEC is piloting production of films that are effective radiators of energy in space, capable of cooling even in direct sunlight. The Center intends to spin off a start-up company to pursue commercial development of these films.
- The Colorado School of Mines ReNUWIt Center carried out numerous STEM outreach
 activities to K-12 students and teachers in the front-range counties, focusing on energywater systems. Pre-college and community college education affiliates include Adams
 County District 50, Denver Public Schools, Englewood Public Schools, Jeffco Public
 Schools, and Shelton Elementary School.
- The ReNUWIt Center collaborates with the City and County of Denver, the Urban Drainage and Flood Control District and Enginuity Engineering Solutions to evaluate impacts on urban flooding.

During calendar year 2016, the Authority received a single distribution of Limited Gaming Funds of \$2.1 million. Interest earnings on those funds totaled \$32,899, for a total income of \$2,132,899 in 2016. Payments to institutions are shown in the table in Appendix A. Total expenses were \$1,987,608.

Please contact me if you have any questions.

Sincerely,

Joe Garcia, Chair

Attachments:

Appendix J:

Spectroscopy Facility

Appendix A: CHECRA Expenses 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 MRI: Inductively Coupled Plasma Dry Etching System for Highly Controlled Etching of Chalcogenides and Related Compounds Appendix E: Colorado State University Accelerating Innovation Research – Research Alliance (AIR-RA) Appendix F: Colorado State University High Energy Physics Accelerator Appendix G: Colorado School of Mines Institute for Advanced Composites Manufacturing Innovation Appendix H: Colorado School of Mines Water Quality and Supply Impacts from Climateinduced Insect Tree Mortality and Resource Management in the Rocky Mountain West Appendix I: Colorado School of Mines Re-inventing the Nation's Urban Water Infrastructure (ReNUWIt) Engineering Research Center

Colorado School of Mines MRI: Environmental X-ray Photoelectron

Appendix A

Colorado Higher Education Competitive Research Authority Summary of Financial Activity - Calendar Year 2016

Balance Available January 1	4,899,101.05
Revenues	
Limited Gaming Fund	2,100,000.00
interest earnings	 32,898.50
Total Revenues	\$ 2,132,899
Disbursements	
Colorado State University	
AIR-RA program	132,000.00
\$400,000 in total; \$134,000 per year 3 years	
DOE Accelerator	90,000.00
\$90,000.00 in total	
Colorado School of Mines	
Engineering Research Center Reinventing Urban Water ERC (renewal) \$400,000 per year/5 years	400,000.00
NSF WSC Category 2 Collaborative	75,000.00
\$75,000 per year/5 years	75,000.00
Advanced Composite Manufacturing Innovation	
\$200,000 per year 5 years split \$100,000 each to CSU and Mines	
MRI: Environmental X-ray Photoelectron Spectroscopy Facility for	
Characterizing Active Interfaces	247,050.00
University of Colorado - Boulder	
NSF MRSEC	400,000.00
Soft Materials Research Center Liquid Crystal Frontiers; and, Click Nucleic Acid IRGs \$400,000 per year/6 years	
NSF Science and Technology Center on Real-Time Function Imaging (STROBE) award notification 5 payments of \$400,000	400,000.00
MRI: CU Boulder: Acquisition of an Inductively Coupled Plasma Dry Etching System for Highly Controlled Etching of Chalcogenides and Related Compounds, PI Wounjhang Park	143,558.00
\$478,527.00 in total	-
Total Disbursements	\$ 2,207,608
Balance Available at December 31	\$ 4,824,392

Financial Notes: Department of Higher Education has not received the invoice for audit charges

Appendix B: University of Colorado, Liquid Crystal Materials Research

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 2016 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, THE 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 understanding 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 2016, 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

<u>Research</u> - 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:

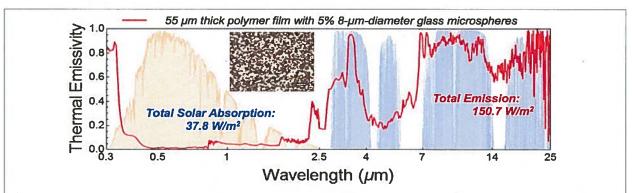
- •Carbon-Edge Resonant X-Ray Scattering from the Twist/Bend Heliconical Structure In 2013, the LCF IRG reported the first visualization of the heliconical structure of the nematic twist/bend (NTB) phase using freeze-fracture transmission electron microscopy, in which the fracture face of a quenched sample is topographically modulated by its intersection with the the helix periodicity. This field-leading effort to structurally characterize the exotic twist/bend liquid crystal phase has recently been extended by our succeeding to make the first in-situ measurements of the bulk helix. Such a study would typically be carried out by x-ray diffraction, but because the NTB helix produces no electron density modulation, its does not scatter x-rays except under resonant conditions. We have applied resonant x-ray scattering at the carbon edge in collaboration with C. Zhu of the Advanced Light Source and have visualized the otherwise invisible NTB helix in CB7CB, CB13CB, and a variety of other TB materials.
- •Diblock Copolymer Click Nucleic Acids After the successful preparation of click nucleic acid homopolymers, we have developed the CNA strategy further to synthesize functionalized CNAs by incorporation of a thiol-functionalized monomer into the polymerization mixture to generate diblock copolymers. We employed poly(ethylene glycol) (PEG) monothiol (Mn~2000) as a model monofunctional thiol, then added the thymine thiol—ene monomer in different stoichiometric ratios. Under typical thiol—ene photopolymerization conditions, the diblock polymer PEG—polyT was prepared. We have thus demonstrated that a simple thiol—ene copolymerization provides a relatively facile method and general approach to functionalize our CNAs.
- •Electrochromic Effects in Anhydrous Thermotropic Liquid Crystal Phases of nanoDNA Liquid crystals are widely used in displays for portable electronic information display. To broaden their scope for other applications like smart windows, new material properties such as polarizer-free operation and tunable memory of a written state become important. Center researchers have developed an anhydrous nanoDNA—surfactant thermotropic liquid crystal system, which exhibits distinctive electrically controlled optical absorption, and temperature-dependent memory. In the liquid crystal isotropic phase, electric field-induced coloration and bleaching have a switching time of seconds. Upon transition to the smectic liquid crystal phase, optical memory of the written state is observed for many hours without applied voltage. The reorientation of the DNA—surfactant lamellar layers plays an important role in preventing color decay. Thereby, the volatility of optoelectronic state can be controlled simply by changing the phase of the material. This research may pave the way for developing a new generation of DNA-based, phase-modulated, photoelectronic devices.
- •Plasmon Enhanced Energy Transfer in Upconversion Nanoparticles One of the most compelling applications of the Center's CNA and DNA nanoconstructions is Energy transfer upconversion (ETU), wherein several low energy photons are combined into a single high energy photon. ETU is known to be the most efficient such upconversion mechanism. Surface plasmons can further enhance the upconversion process, opening doors to many applications. However, ETU is a complex process involving competing transitions between multiple energy levels, and it has been difficult to precisely determine the enhancement mechanisms. We have employed Yb3+ and Er3+ ion doping in the systematic study on the dynamics of the ETU process in nanoparticles deposited on plasmonic nanograting structures. From the transient near-infrared photoluminescence under various excitation power densities, we observed faster energy transfer rates under stronger excitation conditions until it reached saturation where the highest internal upconversion efficiency was achieved. The experimental data were analyzed using the complete set of rate equations. The internal upconversion efficiency was found to be 56% and 36%, respectively, with and without the plasmonic nanograting. We also analyzed the transient green emission and found that it is determined by the infrared transition rate. This is the first report of experimentally measured in-

ternal upconversion efficiency in plasmon enhanced upconversion material, decoupling the internal upconversion efficiency from the overall upconverted luminescence efficiency, allowing more targeted engineering for efficiency improvement.

• Click Nucleic Acid Hydrogels - To demonstrate the capacity of CNA polymers to serve as reversible physical crosslinks, we synthesized a gel structure that utilizes self-complementary pairs of nucleobases [poly(T-alt-A)]. This self-complementary polymer is formed in a single homopolymerization step using a thymine-and adenine-functionalized thiol/allylamineterminated dimer, which was prepared from the thiol-Michael coupling reaction between the thiol of the thymine and the acrylamide of the adenine monomers. MALDI-TOF analysis indicates a 577 Da spacing, which corresponds to the molecular weight of the TA dimer. Although MALDI-TOF accurately determines repeat-unit molecular weights, the molecular-weight averages and distributions determined by this method do not accurately reflect the degree of polymerization because of insufficient ionization in the spectrometer. Furthermore, the Tg of the poly(T-alt-A) polymer was found to be 133°C 8C by DSC. Upon mixing of hybridized CNA- (poly(T-alt-A)) with tetra-PEG-thiol (20 kD) and photoinitiator in DMSO, the specimen remained in a liquid state. After irradiation, which induced the coupling of CNA(poly- (T-alt-A)) to the four-armed PEG core, a CNA-hybridized crosslinked gel was formed as evident from the significant change in viscosity and, ultimately, solidification. The organogel formation was monitored using photorheometry. From the rheological trace, we determined that gelation occurred after 20 s of UV light irradiation. We also performed a control experiment in which a polyT polymer that is not capable of self-complementary binding was coupled to a PEG core with four tetrathiol arms. Whereas there was a change in the mechanical properties upon irradiation, likely owing to hydrophobic interactions after conjugation, the material did not gel (G'<G''), and the elastic modulus was much less than for the CNA(poly(T-alt-A)) crosslinked material. The organogel was also found to be thermoreversible as heating and cooling cycles resulted in obvious viscosity changes. A strain sweep of the organogel revealed a sharp decrease in the modulus at high strains associated with disruption of the CNA(poly(T-alt-A)) crosslinks, elimination of the large strain leads to recovery of the higher modulus associated with reforming of the CNA(poly(T-alt-A)) physical crosslinks. Both reversibility tests and control experiments indicated a non-covalent and sequence-specific interaction that was necessary for organogel formation. For comparison, we also covalently crosslinked an organogel using tetra-PEGSH and tetra-PEG-maleimide, which exhibited a slightly larger elastic modulus than our CNA(poly(T-alt-A)) organogel (ca. 6000 Pa vs. 1000 Pa), likely owing to the reversible nature of the hybridization in the CNA(poly(T-alt-A)) gel as compared with the permanent, covalent crosslinks formed in this type of control gel.

•Nucleic Acid-Assembled Nanoparticles – The size-dependent energy bandgaps of semiconductor nanocrystals or quantum dots (QDs) can be utilized in converting broadband incident radiation efficiently into electric current by cascade energy transfer (ET) between layers of different sized quantum dots, followed by charge dissociation and transport in the bottom layer. Self-assembling such cascade structures with angstrom-scale spatial precision is important for building realistic devices, and DNA-based QD self-assembly can provide an effective assembly route. We are exploring long-range Dexter energy transfer in QD-DNA self-assembled single constructs and ensemble devices. Using photoluminescence, STM spectroscopy, and current-sensing AFM in single QD-DNA cascade constructs, as well as temperature-dependent ensemble devices using TiO₂ nanotubes, we find that Dexter energy transfer, likely mediated by the exciton-shelves in these QD-DNA self-assembled structures, can be used for efficient transport of energy across QD-DNA thin films.

Industrial Outreach - • Polymer/Glass Microsphere Passive Radiative Self-Cooling Optical Metamaterial Films — A glass sphere in a liquid crystal or polymer host Mie scatters and focuses incident light, enhancing the composite's optical absorptivity under appropriate conditions. The Yin group has found that for glass spheres in polymer hosts this effect can lead to films that are transparent in the visible but strongly absorbing in the infrared. If the absorbing wavelength range is the atmospheric transparency window from 7μm to 14μm, such a film near or at room temperature becomes an effective radiator of energy into outer space, capable of cooling itself even in direct sunlight. Pilot production of such films is now operational in Center labs with the intention of spinning off a start-up company to pursue commercial development.



Thermal emissivity vs. wavelength of a polymeric film loaded with glass microspheres. The film is backed with a metal coating that renders it reflective in the visible, and the scattering by the spheres makes it absorbing in the 7 μ m to 14 μ m range of the atmospheric transmission window, also the peak emission wavelength of room-temperature blackbody radiation. The result is a passive optical metamaterial that on a clear day cools itself by infrared radiation, even in direct sunlight.

<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 are:

- •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 2,330 classes have served 89,500 Colorado K-12 students, including 130 classes to 3,500 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 the AY year 2015-16, the Center worked closely with Arrupe's science teacher Stephan Graham to expand its <u>Exploring the Nanoworld MSFCU</u> classroom program with the new theme <u>DNA the Messenger</u>. 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)] met regularly throughout the F15 semester, 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.

Appendix C

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

Total 2016 CHECRA Funding: \$400,000/ Total CHECRA Grant: \$400,000 per year for 5 years

Total NSF Funding for the grant: \$24M over 5 yrs. pending satisfactory progress

Award PI's: Margaret Murnane, Jianwei Miao, Rafael Piestun, Markus Raschke, Naomi

Ginsberg

Project Overview:

Understanding the structure and evolution of matter at the nano and atomic scales is central 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. Indeed, X-ray crystallography has revolutionized many fields of science by determining the three-dimensional (3D) atomic structure of crystals. Transmission electron microscopy (TEM) can routinely resolve atoms in the two-dimensional projection of a 3D crystalline sample. Scanning probe microscopy can image the surface structure at the atomic level. The 2014 Nobel Prize in Chemistry recognized super-resolved fluorescence microscopy, which can generate stunning images of cellular organelles and structures at the nanoscale. However, despite these advanced imaging capabilities, no imaging technique can address some of the most critical questions underlying much of the science and technology in the 21st century. For example, non-crystalline materials such as glasses are ubiquitous in our daily life. Although the history of glassmaking can be traced back to 3,500 BC, the 3D atomic structure of glasses and other disordered materials has thus far defied any direct experimental determination due to its lack of longrange translational and orientational order. On the other hand, much of our modern science and technology relies on non-crystalline systems including renewable energy (amorphous silicon), energy storage (solid electrolyte glasses), telecommunication and computer networking (optical fibers), non-volatile memory (amorphous-crystalline transitions), high efficiency transformers (metallic glasses), information processing (defects and dopants in semiconductors), and biology (cells, cellular organelles, and large protein complexes).

Addressing this grand challenge of imaging non-crystalline, heterogeneous, systems and their dynamics at the on multiple length and spatial scales requires the development of transformative and integrative approaches to imaging science. The STC on Real-Time Functional Imaging (STROBE) has been formed to tackle this major multidisciplinary scientific challenge. In the conventional approach to imaging, scientists from each imaging modality develop standalone microscopes to solve specific scientific problems. In contrast, the STROBE team proposes to advance and integrate different imaging modalities using electron, X-ray, optical and nanoprobe microscopy to collectively tackle major scientific challenges. By taking advantage of their unique expertise in various imaging methods, spanning from atomic resolution electron tomography, to ultrafast X-ray coherent diffractive imaging, and super resolution optical and near field microscopy, the STROBE team will address the following four grand challenges: i) Capturing the 3D position of individual atoms in non-crystalline materials and monitoring their motion; ii) Routine 3D imaging of biological complexes at atomic resolution without the need of crystallization; iii) Real-time functional 3D imaging of energy, magnetic and spintronic materials

at the wavelength limit; and iv) Resolving transport (charge/energy/spin/ions) and fields across interfaces on the nano-scale in amorphous, heterogeneous, and nanostructured materials.

STROBE brings together academe (CU Boulder, UCLA, UC Berkeley, Florida International University (FIU), Fort Lewis College(FLC)), national laboratories (LBL, LANL, NIST), large and small and US industries, as well as international partners, to create and integrate a powerful new set of real-time imaging modalities. CU Boulder leads in ultrafast Xray and visible light sources, which will enable real-time functional 3D X-ray imaging of advanced materials and advanced optical nano-imaging. These will be combined with electron imaging and advanced underpinning technologies to enable integrative approaches for new imaging modalities. UCLA and UC Berkeley will participate in all aspects of the proposed research, while FIU and FLC will participate in visible imaging research. All five campuses will work together to implement, evaluate and disseminate innovative approaches to education, broadening participation and knowledge transfer. Florida International and Fort Lewis College bring strong expertise in education research and outreach as well as an exceptionally diverse student body to the Center. Leaders in imaging science from all partner institutes will improve upon and integrate their expertise to develop unique imaging capabilities with broad application impacting materials science, nanoscience, physics, chemistry, geology, and biology. Leaders in education research will work with an exceptionally diverse team, including several female/Hispanic/Native American scientists. Through an STC, existing strengths will be amplified well beyond the sum of their parts.

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 3 months of STROBE, the following activities benefitted the state –

- The University of Colorado hosted a STROBE Strategic Planning Meeting in October, where 25 university and NSF participants from outside the state joined the local Boulder team members for a 3-day exercise to develop a detailed Strategic and Implementation Plan.
- Ball Aerospace from Boulder joined STROBE as an industry member. Scientists from IBM will visit Boulder for collaborative experiments this summer. STROBE is also characterizing many samples provided by Intel. Other major national companies are also considering membership. These bring many opportunities for students for internship opportunities, permanent positions and for knowledge transfer activities.
- New transdisciplinary graduate programs in imaging science are being developed at CU Boulder, to better prepare students for the 21st century workplace.
- NIST Boulder laboratories will soon start to use STROBE x-ray sources for imaging projects with industry.
- The CHECRA funds are being used for graduate student and postdoc support, as well as for partial support of an experienced Managing Director, who managed a 10-year similar Science and Technology Center in Hawaii (CMORE Center for Microbial Oceanography).
- The Boulder student and faculty team is publishing many top journal articles with industry and national laboratories.

- STROBE provided letters of support to faculty at Fort Lewis College and Mines for large NSF Instrument proposals.
- Several STROBE students won prizes and Fellowships, including graduate student Liz Shanblatt who won the Best Paper Award at the Intnl. Conf. on Computational Imaging; graduate student Maithreyi Gopalakrishna who was recently hired by Intel; and Robert Karl and Charlie Bevis won national NSF and NDSEG Graduate Fellowships.

2/10/17/dc

Appendix D

NSF award to University of Colorado, Boulder (UCB) NSF Award 1625683

Title: MRI: Acquisition of an Inductively Coupled Plasma Dry Etching System for Highly Controlled Etching of Chalcogenides and Related Compounds
Period of Performance 10/01/2016 – 09/30/2019
Total 2016 CHECRA Funding - \$ 143,558
Award PI's – Wounjhang Park, Juliet Gopinath

\$332,961 was awarded by NSF for equipment to UCB. UCB agreed to provide cost share in the amount of \$143,558.

Project Description:

The ability to fabricate high quality electronic and photonic devices has been instrumental in a number of key technology advancements including integrated circuits, solid-state light sources and detectors, energy harvesting, and flexible electronics. In the future, further advancements will lead to miniature optical clocks using chip-scale optical frequency combs, ultra high-speed microprocessors with photonic I/O, high efficiency solar cells with nanopatterned metamaterials, and flexible electronic-photonic devices for biosensing applications. The capability of dry etching with high anisotropy, precisely controlled etch rate and high quality etch surface is critical to most solid-state materials and device research. The objective of this proposal is to acquire an inductively coupled plasma (ICP) dry etching system. Capable of handling multiple gases including chlorine-based gases, the new system is intended to provide etching capability for a variety of materials including compound semiconductors, oxides and metals for which there is no dry etcher available on campus. The new system will also significantly expand the processing capability for silicon. The proposed ICP etcher represents a significant expansion of capabilities in both material types and etch quality. The etcher will spark a wide array of inorganic, organic and hybrid functional materials and devices research, potentially transforming the materials research on campus as well as impacting many research activities in the region and beyond.

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):

The new equipment will be housed in the Colorado Nanofabrication Laboratory and be made available not only to the university users but also to local industry and other research institutions. The capability which is not currently available on campus will enable explorations of new research directions and product developments. Students, both graduate and undergraduate, will learn new skills uniquely provided by the new equipment and will thus be better prepared to find jobs in the leading edge industry or academia. Colorado Nanofabrication Laboratory also host visits by K-12 students and this new state-of-the-art equipment will help attract K-12 students to science and engineering careers.

Appendix E

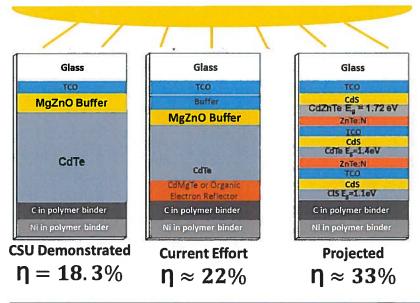
Advanced Thin Film Photovoltaics for Sustainable Energy

NSF AIR:RA Award
Colorado State University
CHECRA Grant (\$400K for 3 years; report covers Years 1 and 2)

Summary: This Accelerating Innovation Research Alliance project proposes to advance both the development of higher-efficiency CdTe based photovoltaic (PV) devices and their timely integration into large-scale manufacturing. The Alliance includes the Next Generation Photovoltaics Center (NSF I/UCRC) at Colorado State University (CSU), the National Renewable Energy Laboratory (NREL), the Center for Renewable Energy Systems in UK (CREST), First Solar and 5N Plus. The center with its research alliance will progress towards its vision of "making PV electricity a major source of energy". The project started on September 1, 2015.

1. Description of the project, the principal persons and the amount of funding:

1a. CdTe Photovoltaics for Sustainable Energy: Energy sustainability represents one of the grand challenges facing modern society, and CdTe thin film solar photovoltaics provide the best opportunity for rapidly expanding renewable energy. CdTe PV is currently competitive for generating electricity in many parts of the world providing electricity at 6-8 US cents/kWh from utility scale projects without subsidy and the costs are decreasing rapidly [Lazard 2014]. Recently an agreement was made to sell electricity from CdTe PV from a new 100 MW field at 3.87 US cents/kWh [Bloomberg 2015]. There are no technical barriers to substantial increase in CdTe PV production. The aim of this project is make CdTe still more cost effective with additional advances. The project will advance CSU's state-of-the-art deposition systems and pursue two separate routes to higher-efficiency manufacturing-friendly cells: (1) Advance the research on Cd1-xMgxTe electron-reflector layer to commercialization, and (2) Optimize PV devices with higher bandgap for multi-junction cells. The roadmap for our center is shown in Figure 1 below:



CSU NGPV's Road Map for High Efficiency Photovoltaics

Figure 1: Efficiency Roadmap for CdTe Photovoltaics at CSU

- **2. Funding from CHECRA and allocation:** The PI for this project is Prof. W. S. Sampath and the Co-PIs are Prof. J. R. Sites and K. L. Barth. The Co-PIs jointly allocate the funding (\$400K for 3 years) from CHECRA. The CHECRA funds have been used to support Dr. Jennifer Drayton; post-doc working and Kevan Cameron; laboratory engineer on the project and for the training of students in the use of advanced materials characterization.
- 4. Results Achieved since September 2015: An advanced co-sublimation vapor source for the deposition of CdMgTe has been designed, fabricated and installed in our research system. This capability is unique and not available elsewhere. Devices with structures shown in the middle in Figure 1 are being fabricated and being optimized. Processing advances have led to the demonstration of device efficiency of 18.3% (independently certified) on low cost soda-lime glass substrates using a low cost sublimation process with two minute cycle time in modest vacuum. Recently a device efficiency of 18.71% was measured in the laboratory. These are the highest efficiency that has been reported for these substrates. Only First Solar has reported higher efficiencies. The device structure and the corresponding current density voltage curve are shown in Figure 2. Also significant progress has been made on solar cells with higher bandgap using CdZnTe. This will be for the device on the top on the right in Figure 1. Passivation of higher bandgap CdZnTe (1.7 eV) was demonstrated and quantum efficiency greater than 70% was demonstrated. This has not been shown before by nay other research group.

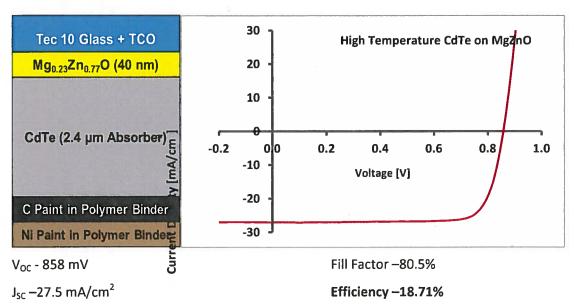


Figure 2: Device Structure for 18.71% efficiency device and the JV curve (J in mA/sq. cm. on the y-axis and volts on the x-axis).

9. References:

Lazard 2014: Lazard's Levelized Cost of Energy Analysis-Version 8.0, published September 2014. Available at http://www.lazard.com

Bloomberg 2015: Bloomberg Business (http://www.bloomberg.com/news/articles/2015-07-07)

Publications since Sept. 2015:

- 1. Sites, J., Munshi, A., Kephart, J., Swanson, D. & Sampath, W. S., (2016, June). Progress and Challenges with CdTe Cell Efficiency, Invited Talk In IEEE 43rd Photovoltaic Specialist Conference (PVSC), June 2016, to be published in the proceedings.
- 2. D. E. Swanson, J. M. Kephart, P. S. Kobyakov, K. Walters, K. C. Cameron, K. L. Barth, W. S. Sampath, J. Drayton, and J. R. Sites, "Single vacuum chamber with multiple close space sublimation sources to fabricate CdTe solar cells," Journal of Vacuum Science & Technology A, vol. 34, no. 2, p. 021202, Mar. 2016.
- 3. Munshi, A, and W. S. Sampath, "CdTe Photovoltaics (PV) for sustainable generation of electricity", invited talk at II VI workshop Chicago, Oct. 7, 2015, and Asian Institute of Technology, March 2016. Also published in Journal of Electronic Materials. 2016 Sep 1;45(9):4612-9.
- 4. Reich C, Swanson D, Shimpi T, Drayton J, Munshi A, Abbas A, Sampath W. Passivation of a Cd 1– x Mg x Te absorber for application in a tandem cell. In Photovoltaic Specialists Conference (PVSC), 2016 IEEE 43rd 2016 Jun 5 (pp. 0487-0491). IEEE.

Appendix F

Report CHECRA grant for the Installation of a liquid Nitrogen delivery line into the Advanced Beam Laboratory at CSU in support of DOE funded research. Principal Investigator: Prof. Jorge J. Rocca

This CHECRA grant (\$ 90,000) makes possible the installation of a liquid nitrogen line in the Advanced Beam Laboratory (ABL) at Colorado State University in support of the research conducted with funding from the US Department of Energy grant "Innovative solutions for scaling high energy femtosecond diode-pumped lasers to multi-kilowatt average power for compact accelerators and application", Principal Investigator Prof. Jorge Rocca, a \$ 1.17 Million project that started in June 2017. The installation will greatly facilitate the delivery of liquid nitrogen for the cooling of cryogenic high average power solid state laser amplifiers that are key for the realization of this project. In addition, the installation will also benefit work conducted with current funding from the National Science Foundation to develop high average power soft x-ray lasers, as well as work done in collaboration with industry, including a Colorado start-up.

The vacuum jacketed liquid nitrogen line funded by the CHECRA grant will connect a 3000 liters liquid nitrogen tank situated outside the ABL Laboratory to liquid nitrogen laser heat exchangers located in a service corridor inside the building. In turn, the heat exchanges will cool high power diode-pumped laser amplifiers. The status of the project is as follows. The design of the liquid nitrogen line was completed, it was approved by CSU facilities, and the order was placed with TECHNI FAB, a manufacturer of cryogenic equipment. Fabrication of the liquid nitrogen line has started at the end of February and installation is scheduled for April, 2017. Full operation is expected by May, when the new capability will make possible the operation of the highest average power high energy ultrashort pulse laser in the world.

The installation will benefit numerous graduate and undergraduate students working in laser development at the Advanced Beam Laboratory. This includes Ph.D students from both the CSU Electrical and Computer Engineering Department and the Physics Department. Involved in the project during the summer will be also additional undergraduate students funded by a National Science Foundation Research Experiences for Undergraduates (REU) site grant (3 years duration) and high school Colorado teachers funded by another 3 year National Science Foundation grant for Research Experiences for Teachers (RET). These teachers will be able to transfer part of the knowledge acquired to their students.

Appendix G

Institute for Advanced Composites Manufacturing Innovation (IACMI)

Colorado School of Mines (CSM)

CHECRA Grant: \$100,000 (per year for 5 years)

Reporting Period: January 1 - December 31, 2016 (BP2)

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 CSM was to contribute to the first two targets in the project, but advances were also made in the area of NDE (item 4). In FY2016 the CSM team made several key contributions to the goal of the wind technology area. The contributions can be summarized in two main areas:

- 1) Design of a mold for test panel fabrication and subsequent mechanical characterization of three different resin systems.
- 2) Design and implementation of experiments to investigate the fundamental properties of the thermoplastic resin system that is a focus of the IACMI project.
- 3) Investigation of viability of biobased thermoplastic resins, phase change materials (PCM), and molecular weight distribution of the thermoplastic resin for use in composites for wind turbine blades

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.

In the present undertaking two commercially available thermoplastic resin systems were evaluated for use in wind blade manufacturing: Nylon-6 and Elium[®]. These resins are commercially available in quantities sufficient to meet the growing wind turbine market needs. Elium[®] is an "acrylate based" system manufactured and sold by Arkema, a partner in the ICAMI project. Like Nylon-6, previous works have shown that Elium[®] parts can also be ground and reprocessed into new parts thus fulfilling the promise of thermoplastics in realizing elements of the so-called circular economy.

In this work, extensive material characterization is performed to assess if property equivalence is observed. Basic mechanical properties of glass fiber reinforced composites, including tensile and compressive moduli and strengths for polyacrylate and polyamide thermoplastic matrices, are indeed equivalent to those of a widely used thermosetting (epoxy) system. However, other physical properties — namely surface tensions, glass transition temperatures, water resistance, viscosity profiles, and heats of reaction are substantially different. Further engineering is needed to enable thermoplastic resin for wind turbine blade.

Principal Senior Investigators

Funding from CHECRA

John R. Dorgan

\$100,000

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

John R. Dorgan: Discretionary funding of promising new research directions including biobased resins, and phase change materials and molecular weight distribution research for exotherm control. Funding for fabrication and mechanical testing of composite panels using thermoplastic resins in comparison with epoxy.

Results achieved

1. Development of panel fabrication mold and subsequent mechanical testing of thermoplastic panels

Panels were fabricated using a light RTM mold from Composites Integration Ltd. (United Kingdom, Ser. No. SO-10302). These 50 cm x 50 cm test panels allowed a vast number of mechanical tests to be conducted on the various resin systems and various fiber layup geometries. In total, 240 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) and three resin systems (i.e., epoxy, Elium[®] and Nylon-6). Specimens were tested in both tension and compression. The results of this study indicated that the thermoplastic matrices of Elium® and Nylon-6 are suitable for wind turbine blade applications when compared with the mechanical properties of epoxy. The conclusion reached at the end of the BP2 was to continue with the Elium® system for wind turbine blade application, but to discontinue the Nylon-6 research. The Nylon-6 system was discontinued over concerns for prohibitively expensive high-temperature tooling and also moisture sensitivity that is inherent in these resin systems. As proof of concept for the Elium[®] resin system for use in wind turbine blades, the IACMI team (Arkema, Johns Manville, NREL) fabricated a 9-meter-long wind turbine blade using Elium® as the resin system. This is the largest blade component made using this resin system to date.

2. Characterization of fundamental properties of the thermoplastic resin system

Several experiments were designed over the course of the last year by the Ph.D. and post-doctoral researchers at the Colorado School of Mines. These experiments and the data that they collect should prove invaluable for design and manufacture of wind turbine blades components in the future budget periods for this project. These experiments include:

a) Characterization and modeling of the exothermic temperature profile of reacting

Elium® during the polymerization

A valuable, yet simple and inexpensive experiment was designed and implemented to characterize the temperature profile of the Elium[®] resin during cure. The reaction was conducted in a 25 ml scintillation vial placed in a constant temperature oil bath. The temperature was measured and collected with thermocouples and data logger. In addition, the surface temperature of open bagged VARTM mold as a function of time was recorded using an IR camera. It is critical to keep the temperature of the resin below the boiling point of the monomer during the cure cycle so as not to boil the monomer which causes voids in the composite part. In parallel, a mathematical model was developed by combining reaction kinetics and heat transfer equation. Total of 6 coupled differential equations with 14 parameters and 22 constants are implemented to Wolfram Mathematica®. The heat transfer coefficient and adjustable parameter for initiator efficiency are determined from the experiment. The developed model reasonably capture the induction time and the maximum temperature. The form and parameters for the model have been shared with Purdue University and Convergent (both are IACMI members). They are currently working with implementing the model to their simulation software (RAVEN®).

b) Development of a chemorheological technique to measure the rheological properties of the curing resin system

First, the viscosity of the Elium® was measured in a cone and plate rheometer as a function of shear rate and temperature. The conclusion of this brief study is that the Elium® resin does not exhibit shear thinning under normal conditions for Vacuum Assisted Resin Transfer Molding (VARTM). Additionally, the parameters for the temperature dependence of the viscosity are to be used in commercial software for modeling the infusion process for these reactive liquid systems. Chemorheology (also referred to as rheokinetics) refers to the in-situ rheological characterization of a polymerizing system. Chemorheological characterization for thermosetting systems is a well-established field, but that concerning thermoplastic polymers is much more limited. In this technique, a radical polymerization is initiated in the Elium[®] using 2 PPHR Luperox AFR-40, Arkema's commercial benzoyl peroxide initiating system. In addition to the rheological properties, this technique allows measurement of the shrinkage of the curing resin system by allowing the top plate of the plate-plate rheometer to "float" on the specimen. Characterization of the cure shrinkage will be critical in specific design engineering for fabricating megawatt scale wind turbine blade components as part of BP4 (2018).

c) Development and utilization of a dual energy X-ray computed tomography scan procedure and a scanning acoustic microscopy procedure for composite void detection

Because the existence of voids may significantly reduce their mechanical properties of fiber reinforced composites (FRCs), it is of great importance to characterize and minimize the voids. Especially, in the case of thermoplastic composites via reactive processing, the temperature of resin may locally exceed its boiling point due to the highly exothermic curing reaction. For each of the panels fabricated, a scanning acoustic microscopy image was taken from a representative section of the panel to investigate the presence of voids. Few if any void structures were seen in the images

generated from scanning acoustic microscopy. However, another technique was developed for using dual energy X-ray computed tomography (CT) to detect the presence of voids in the composite specimens. Dual energy CT scanning allows much better resolution (sub-micron level) and the distinction between air (voids), polymer (resin), and the glass fibers than that provided by acoustic microscopy or even single energy X-ray CT scans. The results show not only spherical voids in the matrix but also irregularly shaped voids because of the physical contact to fibers. This information can be utilized to optimize the processing conditions and sizing chemistry of the fibers. It is recommended that BP3 plans include examining how the annealing temperature affects the voids sizes and shapes. In addition, future work should include dual energy CT measurements during the mechanical load.

3. Investigation of viability of biobased thermoplastic resins, phase change materials (PCM), and molecular weight distribution of the thermoplastic resin for use in composites for wind turbine blades

The utilization of renewable resources in the production of plastics is generally recognized to produce materials with lower embedded fossil energy content and reduced greenhouse gas emissions. In BP2, the CSM group successfully developed a biobased methacrylate resin system that can be used for fabrication of composite parts. However, due to inherent issues with the moisture sensitivity of the polymer used, this portion of the project has been discontinued for further research in the IACMI project. This technology certainly holds great promise in other areas, however, and this preliminary study serves as a launch point for future investigation. Additionally, phase change materials (PCMs) are shown to provide a means of controlling exotherms during composite manufacturing. Importantly, this innovation is demonstrated not only for thermoplastics but also for thermosets thereby providing a means of reducing cycle times regardless of the matrix material. Lastly, the CSM team demonstrated that the molecular weight distribution of the pre-formed polymer added to the resin can drastically affect the exotherm profile for the curing resin. This consideration will be valuable in fine-tuning the Elium® resin system in the BP3 and BP4 projects.

Publications in 2016:

• D. S. Cousins, C. Lowe, D. Swan, R. Barsotti, M. Zhang, K. Gleich, D. Berry, D. Snowberg, and J. R. Dorgan. "Miscible blends of biobased poly(lactide) with poly(methyl methacrylate): Effects of chopped glass fiber incorporation". Accepted to *Journal of Applied Polymer Science* January 2017.

Education and Outreach - Partial CHECRA Support

In 2016, the ICAMI project at the school of mines helped support one post-doctoral research associate, two additional research associates, one Ph.D. graduate student, three hourly undergraduate students, and two summer undergraduate students. 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 (ICAMI meeting held February 1-2, 2017 in Denver, CO)
- 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 utilization of the School if Mines' extensive background in polymer science and state of the art facilities for mechanical testing

Appendix H

Integrated GroundWater Modeling Center (IGWMC)

Colorado School of Mines

CHECRA Grant: \$75,000 (per year for 5 years) Reporting Period: January 1-December 31, 2016

Summary: IGWMC received \$2.3 million from the National Science Foundation to examine the impact of the pine beetle devastation on vital watersheds in the Rocky Mountain west. The project is led by the Colorado School of Mines, in collaboration with research partners from Colorado State University. The study examines the potential water resource changes resulting from the mountain pine beetle epidemic by examining changes in climate, forested ecosystems altered by pine beetle impacts, biogeochemical processes and resource management practices.

(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:

Mountain headwaters in the western United States provide drinking water for more than 60 million people, as well as a broad range of agricultural, ecological, tourism, and industrial water users. The Platte and Colorado River basins alone provide water to more than 30 million residential users and 1.8 million acres of irrigated agriculture. A warming trend in the region has been accompanied by unprecedented tree mortality associated with the ongoing mountain pine beetle (MPB) epidemic, and the ramifications of this event on our water resources are not well understood. The goal of our proposed work is to determine potential water resource changes resulting from the MPB epidemic by defining feedbacks between climate change, insect driven forest disturbance, biogeochemical processes and management practices. This is accomplished with laboratory and field studies that feed fully-coupled, regional hydrologic and climatic models to interpret observations and assess management options that are developed through engaging stakeholders.

In addition to directly affecting the hydrologic cycle, climate change increases ecosystem susceptibility to stressors. Warmer winter minimum temperatures and persistent drought conditions have contributed to the ongoing MPB epidemic in the Rocky Mountains that has affected an estimated 4 million acres of lodgepole pine forests. Subsequent insect-induced stressors, such as the emerging engraver and twig beetle populations threatening young trees, are evidence of the long-term nature of this issue. Large-scale forest disturbances due to beetle-killed forests, as well as forest management practices, can significantly alter watershed hydrology, including evapotranspiration, infiltration, runoff and surface energy fluxes in a region where snowpack is a critical water storage component. We address these land cover perturbations to the hydrologic cycle across a range of scales (hillslope, watershed and regional) using a combination of integrated hydrologic models, hydrologic-atmospheric models and observations.

Just as importantly, soil-vegetation disturbances from beetle-killed forests or forest management may also impact water quality by increasing particulate transport through erosion, increasing nitrification rates and organic carbon fluxes, which can cause decreased soil solution pH, and increasing mobilization and subsequent leaching of metals and metalloids. Similarly, increases in dissolved organic carbon (DOC) in the water supply may lead to increased formation of drinking water disinfection byproducts such as U.S. EPA regulated compounds trihalomethanes, haloacetic acids and nitrosamines. These potential impacts of climate change, beetle-killed forests and management practices on water quantity and quality pose significant threats to public health and the regional economy. In order to accurately assess anthropogenic impacts on hydrology and water resources in mountain watersheds an integrated approach must be taken that accounts for interactions and feedbacks not just within the hydrologic cycle but also between the

natural (climate, hydrologic, ecological and biogeochemical) and human (water and forest management) factors that influence water quantity and quality. To directly address the impacts of changing land cover on the fate and transport of metal and organic compounds we employ field and laboratory studies and reactive transport simulations.

Principal Investigators	Funding from CHECRA
Reed Maxwell, Director and Project Lead for Coupled Modeling	\$713
Jonathan Sharp	\$0
John McCray	\$37,644
Alexis Navarre-Sitchler	\$3,193
Total Spending (Jan. – Dec. 2016)	\$41,550

Students and Postdocs (* funded through CHECRA)

, , ,	Research
	Hydrological effects of forest transpiration
	loss in bark beetle-impacted watersheds
CSM postdoctoral research fellow	Bark beetle infestation impacts on nutrient
	cycling, water quality and interdependent
	hydrological effects
CSM graduate student	Modeling an idealized domain with
(completed PhD in May 2016)	homogeneous forest land cover and a
	heterogeneous subsurface representation
	of a Rocky Mountain watershed
CSM graduate student	Metal cycling in Mountain Pine Beetle
	impacted watersheds
CSM graduate student	Soil microbial nutrient cycling and
(completed MS in Dec 2016)	impacts on carbon and nitrogen outputs
CSM graduate student	Drinking water quality impacts
CSM graduate student	Development and implementation of a
	methodology to produce an enhanced land
	cover product of the Rocky Mountains.
	Development of statistical framework to
1	analyze water quality of stream networks
	in the Rocky Mountains
CSM graduate student	Water-land-atmosphere connections
(completed MS in Dec 2016;	1
transitioned to PhD program)	
CSM graduate student	Field characterization of soil
(completed MS in Dec 2016)	mineralization
0014	T-1 1 1 1 1
CSM research associate	Education and outreach
	CSM graduate student CSM graduate student (completed MS in Dec 2016) CSM graduate student (CSM graduate student CSM graduate student CSM graduate student CSM graduate student CSM graduate student (completed MS in Dec 2016; transitioned to PhD program) CSM graduate student (completed MS in Dec 2016)

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

Reed Maxwell: Travel support for one graduate student at CSM: Nicole Bogenschuetz (MS student, HSE). Nicole completed her MS in December 2016, examining the effect of the Mountain Pine Beetle on stability, soil moisture distribution and root strength in beetle-infected mountain slopes. Prof. Maxwell also supervised student Jefferson, who completed her PhD in May 2016, and Dr. Bearup (completed postdoc). Prof. Maxwell is currently supervising student Forrester, Dr. Gallagher, and Dr. Morse.

John McCray: Partial summer salary for Prof. McCray, RA tuition, fees, stipend, travel and research supplies for Nicolas Rodríguez-Jeangros. Prof. McCray is supervising PhD student Nicolas Rodríguez-Jeangros, working on the development and implementation of a methodology to produce an enhanced (high resolution and frequency) land cover product of the Rocky Mountains. He is also working on the development of a statistical framework to analyze the water quality of the stream networks in the Rocky Mountains.

Alexis Navarre-Sitchler: Partial summer salary for Prof. Navarre-Sitchler. Prof. Navarre-Sitchler is supervising PhD student Elanor Heil, studying metal cycling in mountain pine beetle impacted watersheds.

(c) The results achieved by the project:

Multiscale modeling results:

In order to examine the extent to which MPB-induced transpiration losses can perturb near-surface atmospheric conditions, the Weather Research and Forecasting (WRF) model, a mesoscale meteorological model, was fully coupled to ParFlow (PF), an integrated surface and groundwater hydrologic model. The resulting PF-WRF model was run over the Colorado headwaters, a region devastated by MPB ecohydrological effects, using a method that allows for some representation of initial condition uncertainty in atmospheric modeling. PF-WRF coupled simulations were run with scenarios intended to represent the change that healthy forests undergo as transpiration ceases following MPB infestation ("green" phase and "grey" phase). Comparisons between green and grey phase scenarios support previous literature that shows MPB-induced reductions in evapotranspiration, energy repartitioning, higher water tables and even higher planetary heights. We find significant damping from local to watershed scale, with the addition of un-forested or un-impacted regions. Diurnal signals play a significant role in this dampening, by lagging the response as disturbance moves from surface to atmosphere. Although infestation-induced perturbations to convection and precipitation are insignificant compared to ensemble spread, we find that both energy and atmospheric processes are most sensitive to disturbance in regions with high (shallow) water tables. In fact, when the PF component is removed, WRF's simulated energy and atmospheric processes show much greater impacts from MPB. These results imply that the representation of groundwater, and specifically dynamic subsurface hydrology at depth, affect the response intensity of a major land disturbance event, a finding that has implications to computational hydrology and meteorology.

Additionally, we have recently evaluated the sensitivity of transpiration and stomatal resistance estimates to specified input vegetation parameters. The sensitivity analysis used outputs from an idealized ParFlow-Common Land Model (PF-CLM) domain with homogeneous forest land cover. Parameter sensitivity was shown to vary seasonally and diurnally. Estimates were most sensitive to input parameter values during summer midday hours. Understanding how input parameters influence modeled estimates of transpiration are important since this flux is significantly altered and eventually shutdown as a result of the mountain pine beetle infestation.

PhD Student Nicolas Rodríguez-Jeangros, Professor Amanda Hering, Dr. Tim Kaiser and Professor John McCray developed a statistical methodology for fusing multiple land cover products with different classifications, resolutions, and frequencies into a single land cover product (Spatiotemporal Categorical Map Fusion – ScaMF). The classification, resolution and frequency of the resulting product is an input of the methodology. SCaMF can also be applied to any other spatial categorical data such as soil types. Additionally, SCaMF is also suitable for the down/up-scaling of a single categorical map.

The study of water quality in a changing environment (MPB infestations) requires first a detailed characterization of this environment in space and time. Land cover is a critical variable driving many hydrological processes, so its assessment, monitoring, and characterization are essential inputs to study these processes. However, existing land cover products, derived primarily from satellite spectral imagery, each have different temporal and spatial resolutions and different land cover classes. Therefore, ongoing research is focusing on the implementation of SCaMF over the Rocky Mountains to produce an enhanced land cover product over a period of 30 years with 50-meter spatial resolution and yearly frequency. This project has been implemented using the supercomputing facilities from Colorado School of Mines (BlueM) and NCAR (Yellowstone). A simulation of a full map of the Rocky Mountains represented the largest simulation ever run in BlueM with 512 nodes and 32 tasks per node, resulting in 16,384 tasks with 163,840 simultaneous open file descriptors and a nearly linear speedup. PhD Student Nicolas Rodríguez-Jeangros presented this project at the RMACC symposium earning the 3rd place in the RMACC High Performance Computing Symposium poster competition (2016), which allowed him to also present this project at The International Conference for High Performance Computing, Networking, Storage and Analysis (2016). SCaMF also received an honorable mention from the ENVR Student Paper Award from the American Statistical Association.

Nicole Bogenschuetz defended her Master's thesis, where she investigated the effect of MPB on root strength and soil moisture content, and their subsequent impact on slope stability in mountainous areas. Tensile strength of green- and grey-phase lodgepole pine roots was tested in the field, *in-situ*. The green-phase, or healthy pines, showed a larger tensile strength than the grey-phase pine trees, showing that root strength can be lower in beetle-killed tree stands. ParFlow was used to simulate water table and soil moisture fluctuations on theoretical hillslopes with different inclinations (5, 10, 20 and 30 degrees) and Leaf Area Indices (LAI's) related to healthy, green-phase forest coverage and beetle-killed grey-phase forests. Overall, soil moisture content was found to be greater in grey-phase beetle-killed hillslopes, and increased with decreasing slope inclination. Both the tensile strength and hydrologic results were input to a two-dimensional infinite-slope stability model to test for the combined effect of reduced root strength and increased soil moisture content – two trends that tend to increase susceptibility for slope failure. A slope's factor of safety was found to have decreased most prominently on slopes with the lowest inclinations (5 - 10 degrees), and factor of safety changes were most closely related to hydrologic changes in the soil, not changes in root strength. The findings in this study are currently being developed for a paper to be submitted to a peer-reviewed journal.

Biogeochemical field and laboratory results:

Investigation of seasonal water quality in watersheds displaying varying levels of bark beetle infestation revealed that organic carbon concentrations, aromatic character and disinfection byproduct formation potential were elevated in waters sourced from high beetle-impacted watersheds compared to moderate and low impact watersheds. Beetle impact was found to exasperate seasonal increases in carbon loading and disinfection byproduct formation potential following both runoff and precipitation events. These findings have been synthesized and are now published in Science of the Total Environment (Brouillard et al). Shifts in soil properties and bacterial communities were observed under different tree phases at a highly beetle impacted site (>80%) but not at one with less impact (<20%). Microbial diversity increased in soils under beetle impacted trees and correlates to shifts in organic matter properties. The emergence of bacterial clades more adept at degrading refractory carbon were found to increase with beetle impact. These findings have been published in the journal of Soil Biology and Biogeochemistry (Mikkelson et al). In addition to looking at soil properties and bacterial community shifts beneath beetle-killed trees, we have analyzed which bacterial communities are metabolically active and which are dormant throughout this disturbance. Results suggest that rare taxa are able to transition to dormancy during large-scale tree

mortality maintaining overall community diversity and contributing disproportionately to community dynamics. This research is now published in Applied and Environmental Microbiology (Mikkelson et al).

In order to investigate the variability in biogeochemical response observed at the two sites mentioned above (high beetle impact and less beetle impact), we established a field site with beetle-killed trees surrounded by varying levels of tree mortality. Soil respiration was significantly lower under beetle-impacted trees compared to live trees and related to the number of live trees within each study plot. Additionally, we observed a threshold response in the upper horizons with respect to ammonium, which accumulated only under trees surrounded by at least 40% tree mortality. Concurrently, C:N ratios decreased as the extent of surrounding tree mortality increased and ammonium only accumulates at low C:N ratios. The ammonium threshold is related to the extent of surrounding tree mortality and the C:N ratio, suggesting that soil N-cycling is altered to favor inorganic, mobile forms of N when there are high levels of tree mortality and the soil environment shifts from N-limitation to N-saturation. This research has recently been submitted to peer review.

In evaluating the relationships between insect-induced tree mortality and fire severity, results demonstrate that forest fires do not burn more severely in beetle-impacted areas than in un-impacted forests. Contrary to public perception, Mountain Pine Beetle infestation was actually found to reduce fire severity across the Western US compared to un-impacted pine forests. This effect was more pronounced for Lodgepole pine host species than ponderosa pine species. The conclusions of this study may aid in forest management and policy decisions while reducing unintended secondary effects associated with tree harvest following infestation. Efforts on this topic are currently focusing on manuscript preparation and submission. In a complementary project, work began near Crested Butte to better understand how various climate change variables of temperature, moisture and bark beetle-induced tree mortality affect needle decay processes and the associated release of carbon and nitrogen in the environment. Various types of beetle impacted and non-beetle impacted needles were deployed along Washington Gulch to study biogeochemical cycling and decay that results from needle imports on designated plots of land. Temperature and moisture will be monitored throughout the field plots. In addition, needle chemistry content changes will be monitored directly with sacrificed needles from the field plots and with archived needles stored on campus. Sampling events to study biogeochemical processes and decay will also occur on site to test C:N cycling in the subsurface hydrosphere with lysimeters and the atmosphere with a Picarro gas analyzer.

To evaluate metal mobility, four watersheds along Keystone Gulch Rd., located in Keystone, CO, were chosen for soil and water sampling because of their similar bedrock, drainage area, tree density and type, aspect and their varying degree of pine beetle infestation. Sequential extractions using simulated rainwater, MgCl₂ and pyrophosphate (representing soil pore water, exchangeable fraction and organically bound metals) were performed on the Keystone Gulch soil samples to develop a better understanding of the distribution of metals in soils. At the watershed scale, soil pH and total carbon were not dependent on total beetle kill. Statistical analysis of metals from labile, exchangeable and organically bound fractions of soils collected from multiple pits within the four different watersheds showed that there is no significant difference in metal availability as a function of watershed scale beetle kill. Differences in watershed scale metal availability were dominantly a function of horizon and total carbon.

(d) Education and outreach activities:

Prof. Maxwell, along with Dr. Gallagher and Dr. Morse (Prof. Navarre-Sitchler and Prof. Sharp also taught 1 lecture each) taught an honors course in Fall 2016 entitled, "Naked Trees, Killer Beetles, and Dirty Water." This was a collaborative honors course at Colorado School of Mines (CSM) and Colorado State University (CSU) that examined current physical and social science research on the effects of the

Mountain Pine Beetle on regional social and ecological systems in the Rocky Mountain West. Undergraduate honors students became beetle experts, then used their expertise to develop lessons and activities for 6th grade students at Windy Peak Outdoor Lab (Jefferson County, CO Schools; Bailey, CO). The content developed for outreach in this course is being incorporated into the curriculum at Windy Peak, impacting around 6,000 students each year. The course was well received by all involved parties and plans to offer the course again in fall 2017 are underway.

Additional K-12, university, and professional education outreach activities resulting from this project include:

- Dr. Morse and Dr. Gallagher spoke to a group of high school students on a campus tour about the hydrological science and engineering program at CSM, and demonstrated hands-on hydrology concepts (D'Evelyn HS; March 2016).
- Dr. Morse, Dr. Gallagher, MM Forrester--Math and science events at three local elementary schools (9/27/16 Mitchell Elementary; 11/2/16 Shelton Elementary; 11/30/16 Edison Elementary) At these events, students are taught elements of the water cycle and how water and contaminants move through the natural environment using a variety of visual and interactive activities.
- C Bokman, B Brouillard, Prof. Sharp—Mitchell Elementary Math and Science Night; Microscopy and Enviroscape Modules (9/27/16).
- Dr. Morse and Dr. Gallagher attended River Watch Colorado training, where volunteer groups from across Colorado become "citizen scientists" by monitoring water quality parameters that are used by the state for regulatory decisions.
- Dr. Gallagher visited Alameda International high school and talked to 6 high school science classes about careers in Geosciences and the Mining for Talent field trip (11/8/16).
- Dr. Gallagher collaborated with Prof. Singha (not on project) to develop and organize the Mining for Talent event, a field trip opportunity for high school students. Applicants have an opportunity to tour CSM campus, visit labs to understand ongoing research in geosciences, and participate in lab experiments to teach them about techniques used in geology, hydrology, and other fields. The first event was in March 2016 and was so successful that a second event was hosted in December 2016. Prof. Sharp provided lab access to student group, as well as microscopy-based lab activities.
- Prof. Sharp and B Brouillard judged an Elementary Science Fair March 2, 2016 at Mitchell Elementary
- Prof. Sharp—Environmental Learning for the Future (ELF) Program Instructor, Mitchell Elementary with targeted hands-on delivery to K-5 students (~4 modules).
- Prof. Sharp—REU mentorship for undergraduate student Laura Leonard, investigating facets of microbial processes and mountain pine beetle geochemistry; she is now a graduate student.
- Prof. Sharp—RET mentorship and hosting for middle school teachers Renee Lee and Melissa McVey during June/July 2016
- Prof. Sharp—Development and delivery of 4 hands-on microbiology tutorials for 8 RET teachers. Modules were designed to enable teachers to deliver material in the classroom and develop lesson

plans around the broader themes: 1) Winogradsky columns 2) DNA extraction 3) Microscopy 4) PCR amplification/DNA visualization.

Publications:

Bearup LA, RM Maxwell and JE McCray (2016) Hillslope response to insect-induced land-cover change: an integrated model of end-member mixing. *Ecohydrology*, 9: 195-203. DOI: 10.1002/eco.1729.

Brouillard BM, ERV Dickenson, KM Mikkelson and JO Sharp (2016) Water quality following extensive beetle-induced tree mortality: Interplay of aromatic carbon loading, disinfection byproducts, and hydrologic drivers. *Science of the Total Environment. In press.* DOI: 10.1016/j.scitotenv.2016.06.106.

Jefferson JL, RM Maxwell and PG Constantine (2017) Exploring the sensitivity of photosynthesis and stomatal resistance parameters in a land surface model. Journal of Hydrometeorology. Vol. preprint. DOI: 10.1175/JHM-D-16-00531.

Mikkelson KM, CA Lozupone, and JO Sharp (2016) Altered edaphic parameters couple to shifts in terrestrial bacterial community structure associated with insect-induced tree mortality. *Soil Biology and Biochemistry* 95, 19-29.

Mikkelson KM, C Bokman and JO Sharp (2016) Rare taxa maintain microbial diversity and contribute to terrestrial community dynamics throughout bark beetle infestation. *Applied and Environmental Microbiology*. AEM. 02245-16.

Penn CA, LA Bearup, RM Maxwell and DW Clow (2016) Numerical experiments to explain multiscale hydrological responses to mountain pine beetle tree mortality in a headwater watershed. *Water Resources Research*, 52: 3143-3161. DOI: 10.1002/2015WR018300.

Rodríguez-Jeangros N, AS Hering, T Kaiser and JE McCray (2016) Fusing Multiple Existing Space-Time Land Cover Products. *Environmetircs*. DOI: 10.1002/env.2429.

Presentations:

Bearup LA, C Penn, N Engdahl, JE McCray and RM Maxwell. Hydrologic response to widespread land cover change simulated from the hillslope through the regional scale. Poster presentation at the NSF Water Sustainability and Climate PI Meeting, Arlington, VA. March, 2016.

Bogenschuetz N, LA Bearup, RM Maxwell and P Santi. The Effect of the Mountain Pine Beetle on Slope Stability, Soil Moisture, and Root Strength. Poster presentation at the Colorado School of Mines Geology and Geological Engineering Research Fair. Golden, CO. February, 2016.

Bogenschuetz N, LA Bearup, RM Maxwell and P Santi. The Effect of the Mountain Pine Beetle on Slope Stability, Soil Moisture, and Root Strength. Poster presentation at the NSF Water Sustainability and Climate PI Meeting, Arlington, VA. March, 2016.

Bogenschuetz N, AL Bearup, RM Maxwell and P Santi. The Effect of the Mountain Pine Beetle on Slope Stability, Soil Moisture, and Root Strength. Poste presentation at the Colorado School of Mines Graduate Research and Discovery Symposium. Golden, CO. March, 2016.

Bokman CM, BM Brouillard, KM Mikkelson and JO Sharp. Altered nutrient cycling and microbial drivers after mountain pine beetle infestation. Poster presentation at the NSF Water Sustainability and Climate PI Meeting, Arlington, VA. March, 2016.

Brouillard BM, ERV Dickenson, KM Mikkelson and JO Sharp. Enhanced aromatic carbon loading, DBP formation potential, and hydrologic variability following beetle-induced tree mortality. Poster presentation at the NSF Water Sustainability and Climate PI Meeting, Arlington, VA. March, 2016.

Brouillard BM, CM Bokman, KM Mikkelson and JO Sharp. Shifts in geochemical parameters and greenhouse gas fluxes following insect-induced tree mortality. Poster presentation at the American Geophysical Union annual meeting, San Francisco, CA. December 2016.

Forrester MM, RM Maxwell, LA Bearup, D Gochis and A Porter. Exploring atmospheric feedbacks from large-scale land disturbance with a coupled hydrologic-atmospheric model. Poster presentation at GRADS Research Fair, Colorado School of Mines, Golden, CO. March, 2016.

Forrester MM, RM Maxwell, LA Bearup, D Gochis and A Porter. Exploring atmospheric feedbacks from large-scale land disturbance with a coupled hydrologic-atmospheric model. Poster presentation at the NSF Water Sustainability and Climate PI Meeting, Arlington, VA. March, 2016.

Forrester MM. Ecohydrologic response and atmospheric feedbacks from beetle-induced transpiration losses in the Colorado headwaters. Oral presentation at the American Geophysical Union annual meeting, San Francisco, CA. December, 2016.

Gallagher LK, MS Morse and RM Maxwell. Using the mountain pine beetle infestation of the Rocky Mountain West to develop a collaborative, experiential course on science communication. Poster presentation at the American Geophysical Union annual meeting, San Francisco, CA. December 2016.

Heil E and A Navarre-Sitchler. Metal cycling in mountain pine beetle impacted watersheds. Poster presentation at the Colorado School of Mines Geology and Geological Engineering Research Fair, Golden, CO. February, 2016.

Heil E, A Navarre-Sitchler and RB Wanty. Metal cycling within mountain pine beetle impacted watersheds of Keystone Gulch, Colorado. Poster presentation at the Geological Society of America annual conference, Denver, CO. September, 2016.

Heil E, A Navarre-Sitchler and RB Wanty. Metal cycling within mountain pine beetle impacted watersheds of Keystone Gulch, Colorado. Poster presentation at the American Geophysical Union annual meeting, San Francisco, CA. December 2016.

Morse MS, LK Gallagher and RM Maxwell. Using a WSC collaborative launchpad to advance a comprehensive education and outreach initiative. Poster presentation at the NSF Water Sustainability and Climate PI Meeting, Arlington, VA. March, 2016.

Navarre-Sitchler A, JO Sharp et al. Water quality and supply impacts from climate induced tree mortality in the Rocky Mountain West. Oral presentation at the NSF Water Sustainability and Climate PI Meeting, Arlington, VA. March, 2016.

Rodríguez-Jeangros N, AS Hering, T Kaiser and JE McCray. Spatiotemporal Categorical Map Fusion (SCaMF) – A methodology to fuse multiple categorical maps in space and time using parallel computing. Poster presentation at the American Geophysical Union annual meeting, San Francisco, CA. December 2016.

Rodríguez-Jeangros N, AS Hering, T Kaiser and JE McCray. A parallel implementation of a methodology for fusing existing land cover products. Poster presentation at the RMACC High Performance Computing Symposium, Fort Collins, CO. August, 2016.

Rodríguez-Jeangros N, AS Hering, T Kaiser and JE McCray. A parallel implementation of a methodology for fusing existing land cover products. Poster presentation at the International Conference for High Performance Computing, Networking, Storage and Analysis, Salt Lake City, UT. November, 2016.

Rodríguez-Jeangros N, AS Hering, JE McCray and T Kaiser. Fusing Multiple Existing Space-Time Land Cover Products. Oral presentation at the SIAM Conference on Uncertainty Quantification, Lausanne, Switzerland. April, 2016.

Rodríguez-Jeangros N, AS Hering and JE McCray. Preliminary analysis of the effects of MPB infestations on DOC stream concentrations, and data compilation to extend the spatio-temporal analysis. Poster presentation at the NSF Water Sustainability and Climate PI Meeting, Arlington, VA. March, 2016.

Sharp JO, CM Bokman, BM Brouillard and KM Mikkelson. Increases in terrestrial nitrogen availability and microbial biogeochemical indicators in association with extent of surrounding tree mortality in bark beetle impacted forests. Poster presentation at the American Geophysical Union annual meeting, San Francisco, CA. December 2016.

Appendix I

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, 2016

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.

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 assess 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, fourteen projects were funded in 2015:

- Tools to support decision making for nested, spatially-scaled, integrated urban water infrastructure (U1.2);
- Innovative Stormwater Management in Denver (U2.5);
- Tailoring Water Reclamation for Specific Purposes (E1.1);
- Sustainable landscape irrigation with reclaimed water (E1.5);
- Microalgae for wastewater treatment and recovery: A new approach to onsite wastewater treatment (E2.2);
- Reclaiming Energy from Wastewater using Anaerboic Digestion (E2.4);
- Chemical valorization of Energy from Waste (E2.12)
- Alternative Potable Reuse Treatment Trains (E3.4, new project in 2016)
- Smart Engineered Wetlands (N1.2);
- Managed aguifer recharge and recovery: Simulation, modeling and operation (N2.1);
- Managed Aquifer Recharge for Water Quality (N2.2)
- High Resolution Urban Stormwater Modeling (N3.1);
- 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	\$16,069
Project co-Lead, Innovative Stormwater Management in Denver, U2.5 and	\$41,253
Project co-Lead, Engineering Streambeds for Water Quality Improvement,	
N.3.4	
Tzahi Cath	
Project Lead, Tailoring Water Reclamation for Specific Purposes, E1.1	\$65,793
Linda Figueroa	
Project Lead, Reclaiming Energy from Wastewater using Anaerboic	\$51,423
Digestion, E2.4	
Christopher Higgins	
Project Lead, Stormwater Infrastructure for Water Quality, N3.3	\$6,980
Project co-Lead, Engineering Streambeds for Water Quality Improvement,	
N.3.4	
Terri Hogue	***
Project co-Lead, Innovative Stormwater Management in Denver, U2.5	\$41,253
Reed Maxwell	000 440
Project Lead, High Resolution Urban Stormwater Modeling, N3.1	\$36,143
Jonathan Sharp	A7 000
Project Lead, Smart Engineered Wetlands, N1.2	\$7,203
Project Lead, Managed Aquifer Recharge for Water Quality, N2.2	\$3,571
Timothy Strathmann	#7.000
Project Lead, Chemical valorization of Energy from Waste, E2.12	\$7,203
TOTAL SPENDING (Jan-Dec 2016)	\$269,688

Within the ReNUWIt projects (2016), full or partial support was provided to:

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

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

John McCray, Professor: Discretionary Center funding for supporting new research directions; a stormwater symposium to share research findings with Coloradoans; and travel support for students and faculty. Partial salary support was for ReNUWIt Center management and student advising and mentoring. In support of the Denver Stormwater Planning project (U2.5) CHECRA funding supported one semester of tuition, stipend and nominal materials for a MS student, an undergraduate student to assist with assessment of LID impacts to stormwater, and one teaching faculty for data synthesis in development of engineering drawing at Willis Case Golf

Course. McCray also leads a new project in 2016 (N3.5), which is a partnership with the City of Golden, to engineer streambeds in stormwater channels to improve water quality. Mines and Golden were recently jointly awarded a Mines Proof of Concept (POC) Innovation grant, awarded by an external technical advisory board of Colorado business entrepreneurs.

Tzahi Cath, Associate Professor: Funding for two graduate students focused on SB-MBR energy optimization and tailored non-potable reuse of treated wastewater (E1.1).

Linda Figueroa, Associate Professor: Tuition and stipend support for a graduate student who is continuing work on development a pilot-scale reactor for energy recovery (methane gas) in cooperation with Plum Creek Wastewater Authority, Castle Rock, CO (E2.4). Partial faculty salary support was provided for student advising and mentoring. Nominal funding was used for materials and sample analysis from the pilot scale anaerobic bioreactor at Plum Creek Wastewater Authority.

Christopher Higgins, Associate Professor: Partial support for one post doctoral fellow for work with the City of Denver to develop of a field site at Cuernavaca Park for pilot scale testing of BioCHARGE (N3.3).

Terri Hogue, Professor: One undergraduate student was supported for hydrologic modeling of the Berkeley neighborhood in northwest Denver and partial salary support for Dr. Hogue for student oversight (U2.5). Nominal funds were provided for stormwater quality analyses and supplies.

Reed Maxwell, Professor: One graduate student was supported looking at stormwater flow and quantity impacts of converting pervious areas to low impact development in urbanized watersheds (N3.1). Specifically modeling has evaluated the impacts associated with converting 15%, 25%, 35% and 50% of existing pervious areas under different design storms (2-Yr, 5-Yr, 10-Yr, 50-Yr, 100-Yr) on flooding.

Jonathan Sharp, Associate Professor: Partial faculty salary support was provided for student and research faculty advising and mentoring (N1.2) for engineering smart wetlands designed to remove specific pollutants of interest. Nominal salary support was provided to one research assistant professor to evaluate attenuation of trace organic chemicals in managed aquifer recharge systems (N2.2).

Results Achieved

Center scientists and engineers continued field research at Mines campus test bed that utilizes and treats municipal wastewater (~7,000 gal/day). The demonstration-scale treatment unit 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. Strategies for optimization of generating on-demand effluent qualities with elevated levels of nitrogen while simultaneously optimizing energy demands continue. For example, E2.12 was initiated in 2015 to produce hydrocarbon fuels and chemical intermediates from wastewater biosolids (energy-rich microalgae and PHB rich bacterial solids) via hydrothermal and aqueous catalytic technologies.

Identifying mechanisms by which nutrient removal can efficiently be achieved while lowering energy consumption is beneficial both from an energy resource standpoint and an economic perspective. In addition, a fifth season of fertigation (use of reclaimed wastewater for irrigation to optimize nutrient removal and application) was completed with analyses of leachate, and soil samples collection to assess using tailored water to reduce potable use and mineral fertilizers, and minimize nitrate leaching to groundwater.

Researchers are working to develop 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.

Demonstration scale anaerobic baffled reactors have been operating at the Plume Creek Water Reclamation Authority (PCWRA) in Castle Rock for four 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. The results from primary anaerobic treatment have led to additional investment by NSF and Water Environment Research Foundation (WERF) to enhance our understanding of the fundamental processes in a pilot system with primary and secondary anaerobic treatment stages to be constructed and operated at the Mines Park Test Bed Facility. As a result, project researchers have been solicited by water reclamation utilities in Western States to explore testing and upscaling of the anaerobic mainstream treatment.

Numerous activities have also focused on stormwater capture, treatment and reuse (see attached supplement research project synopses). Development and implementation of a new geomedia (BioCHARGE) is moving forward with field scale testing planned in collaboration with the City of Denver at Cuernavaca Park for removal of stormwater pollutants during infiltration. Stormwater modeling simulations within the South Platte River Basin, southeast of Downtown Denver in Parker provide ultra-high-resolution (1 m extent) detail on water movement on the surface (i.e. routing water from the rooftop to the gutters and into the drains) and subsurface (i.e. routing water through complex layers of biofilters or within BMPs) providing information to municipalities on how design, placement, and material usage of stormwater infrastructure impacts in-situ water quality and peak storm flow mitigation.

CSM center scientists and students also continued collaborations focusing on stormwater planning, management and treatment. In partnership with the City and County of Denver, feasibility analysis and conceptual design for beneficial use of non-potable stormwater in a west Denver neighborhood using regional best management practices (BMPs) is being conducted. Implementation at parks and recreation land would enable potential urban irrigation while meeting water quality standards for discharge into Clear Creek, and stakeholder regulatory and sustainability goals. In another project, we are also working with the USGS National Water Quality Lab, evaluating sources of organic chemicals in urban stormwater, BMPs for removal from urban stormwater, and redesign of bioinfiltration systems to control both the quantity and quality of urban stormwater in Colorado.

In Fall 2016, a Stormwater Symposium was held on the Mines campus to share findings on stormwater research and learn about current practices and issues within the Colorado stormwater sector. Over 50 participants attended from local government and regulatory agencies (City, County, State, and Federal representatives), private industry, non-profit

organizations, and citizen groups. Networking with ReNUWIt students was provided through a poster session.

As noted in 2015, our stormwater research has also enabled us to produce research results that have led to additional funding that is synergistic with our ReNUWIt mission. A new \$2M grant from US EPA was awarded to evaluate the life-cycle performance and costs for green and gray stormwater infrastructure. Denver Water is interested in conducting a study similar to one we currently have with Orange County CA, evaluating the primary factors economic, social, and land-use factors associated with urban water use to inform utilities on effective pricing strategies for water conservation.

Summary of Benefits to the State of Colorado

- Received \$830,000 NSF core funds in 2016. These funds in combination with CHECRA funds (\$400,000) and \$119,401 CSM matching funds have supported:
 - 22 graduate students (tuition and stipend) in the first 5 years of ReNUWIt (2011-2016) with degrees in Civil & Environmental Engineering, Hydrologic Science and Engineering, Geological Engineering, and Applied Math and Statistics. Women comprised ~50% of these graduate students. Most of these students will enter the Colorado STEM workforce.
 - o Research experiences for 22 Mines undergraduates with ~60% of these students female. Again, most of these students will enter the Colorado STEM workforce.
 - Numerous STEM outreach activities to K-12 students and teachers in the front-range counties, focusing on energy-water systems. Pre-college and community college education affiliates include Adams County District 50, Denver Public Schools, Englewood Public Schools, Jeffco Public Schools, and Shelton Elementary School.
- In collaboration with the NREL, we are developing new technologies for producing renewable energy, valuable biorenewable chemicals, and freshwater from municipal and industrial wastewater streams in Colorado.
- In collaboration with Metro Wastewater Reclamation District and Carollo Engineers, we
 are investigating potential energy savings and treatment efficiencies associated with
 alterations in treatment plant operation for nutrient removal. Successful improvements
 lower energy consumption and subsequent application of reclaimed wastewater to
 fertigation decreases the level of nutrient removal required.
- Continued collaboration with the City and County of Denver, the Urban Drainage and Flood Control District (UDFCD), and Enginuity Engineering Solutions, to evaluate how low impervious design (LID) impacts on urban flooding using high resolution models. Recommendations on how the City can incorporate LIDs as a viable alternative in master planning for improved water quantity and quality is planned in 2017 (next year).
- Continued project with the City and County of Denver (U.2.5) that is jointly funded by the City and ReNUWIt. Three M.S. students are working on this project, which is a technical, economic, and legal feasibility study for beneficial stormwater use in a west Denver neighborhood.
- Based on outcomes from E2.4, Plum Creek Water Reclamation Authority is planning to construct a demonstration scale mainstream anaerobic treatment system.
- Engagement of 50+ practitioners from the Colorado stormwater sector during a half-day symposium to exchange ideas and information between Mines students and researchers and stormwater industry at large.

- Presented training to practitioners in the State of Colorado at the lunch and learn series
 of the Colorado Association of Stormwater and Floodplain Managers (CASFM), as well
 as at the annual CASFM conference.
- Bi-monthly seminars organized and sponsored by the ReNUWIt students. Seminar speakers and topics include a range of student research, industry partners, and experts.

Publications in 2016 (funded wholly or in part with CHECRA funds):

Thesis and Dissertations:

- Cherry, Lisa. (2016). Predicting Parcel Scale Redevelopment within the Berkeley Neighborhood in Denver Colorado using Linear and Logistic Regression. M.S. Thesis. Civil and Environmental Engineering, Colorado School of Mines, Golden, CO.
- Coontz, Jason (2106). Influence of MLSS, Aeration, and Mixing on Oxygen Transfer Parameters in a Sequencing Batch Membrane Bioreactor. M.S. Thesis. Civil and Environmental Engineering, Colorado School of Mines, Golden, CO.
- Ulrich, Bridget (2016). Biochar-amended Biofilters for Removal of Trace Organic Contaminants from Stormwater. PhD. Dissertation. Civil and Environmental Engineering, Colorado School of Mines, Golden, CO.

Leveraged with CHECRA but no direct funds:

Billings-Frank, Victoria (2016). Co-Treatment of Domestic and Oil & Gas Wasteater with a Hybrid Sequencing Batch Reactor-Membrane Bioreactor. M.S. Thesis. Civil and Environmental Engineering, Colorado School of Mines, Golden, CO.

Publications:

- Kazor, K.E., Holloway, R.W., Cath, T.Y., Hering, A.S. (2016). Comparison of linear and nonlinear dimension reduction techniques for automated process monitoring of a decentralized wastewater treatment facility, *Stochastic Environmental Research and Risk Assessment*, 30:1527-1544.
- Li D., Sharp J.O., Drewes J.E. (2016). Influence of wastewater discharge on the metabolic potential of the microbial community in river sediments. *Microb Ecol.* 71:78-86.
- Ramey, D.F., Munakata-Marr, J., Cath, T.Y. (2016). Hypoaeration of activated sludge to reduce energy requirements at distributed reclaimed water plants: Studies at bench and pilot scales, *Environmental Science: Water Research & Technology*, DOI: 10.1039/C6EW00208K.
- Riley, S.M., Oliveira, J.M.S., Regnery, J., Cath, T.Y. (2016). Hybrid membrane bio-systems for sustainable treatment of oil & gas produced water and frac flowback, *Separation and Purification Technology*, 171:297–311.

Appendix J

Acquisition of Rocky Mountain Environmental X-ray Photoelectron Spectroscopy Facility of *In Situ* Characterization of Active Surfaces

Colorado School of Mines

CHECRA Grant: \$247,050 (one-time grant) Reporting Period: January 1 - December 31, 2016

Summary: This grant provides cost-share funds for the acquisition of an Environmental X-ray Photoelectron Spectrometer (E-XPS) to establish a unique regional facility for exploring behavior of material surfaces in operating and/or reactive environments and for training in advanced measurements at the Colorado School of Mines (CSM) and collaborating institutions across the Rocky Mountain region.

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: For many functional materials critical to our nation's energy and environmental future, performance depends on material surface properties during device operation, which can vary quite significantly from surface properties under conditions typically measured by standard high-vacuum surface analysis tools (e.g., high-vacuum XPS). The inability for many researchers to study interfacial chemical states during device operation or in relevant ambient conditions presents a substantial barrier to fundamental scientific insight.

For this reason, the E-XPS user facility established in part by this award will enable new insights into in a diverse array of material-dependent technologies and scientific fields. This E-XPS center will significantly expand access for new and interested users across the Rocky Mountain Region in engineering, chemistry, geophysics, and other disciplines to employ E-XPS to study materials and surfaces in active environments. The instrument will be installed and established as a self-sustaining user facility at CSM to advance XPS capabilities in the region for both internal and external users. The established facility will provide world-class material science research and education experiences for the next generation of science and engineering leaders from CSM and elsewhere. The facility will advance students' knowledge of instrumentation, instrument capabilities, sample preparation, and data analysis relevant to their respective fields of study in undergraduate and graduate coursework and research activities,

The E-XPS user facility established by this award will allow measurements of solid-vapor and solid-liquid-vapor interfaces at pressures up to 25 mbar, temperatures up to 800°C, and can operate with electrochemical perturbation of non-equilibrated surfaces. These capabilities enable surface characterization in realistic chemical, electrochemical, and thermal environments for processes related to energy conversion, chemical processing, geochemistry, and materials degradation. The unit can measure lateral or depth profiles in a single spectrum, and can operate under standard XPS (i.e. UHV) conditions, thereby meeting a critical need at CSM.

E-XPS has only recently expanded from heavily oversubscribed synchrotron-based user facilities to laboratory-scale instruments. This user facility will therefore greatly improve access and

throughput for E-XPS capabilities, enabling groundbreaking and collaborative interdisciplinary materials research at CSM and at collaborating regional universities and federal research labs. Expected users from numerous engineering disciplines, physical sciences, and geological sciences will employ the E-XPS instrument to address outstanding questions about material surface behavior in arenas such as energy conversion technologies, geochemistry, environmental processes, and materials fabrication. It is further anticipated that technological implications of these unique measurements in active environments will draw in industrial users in these fields.

The entirety of the grant is applied toward NSF-mandated cost share for purchase of the instrument; no funds are associated with faculty salary or direct research expenditures. That said, the PIs on this NSF-funded grant are listed below. For convenience, the entire CHECRA grant amount is associated with the PI.

Principal Investigators	Funding from CHECRA
Steven DeCaluwe, CSM Principal Investigator	
	\$247,050
Svitlana Pylypenko, CSM co-PI	
Sumit Agarwal, CSM co-PI	
Gregory Jackson, CSM co-PI	
Manika Prasad, CSM co-PI	
TOTAL SPENDING/ENCUMBRANCE (Jan-Dec 2016)	\$247,050

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

The funds have all been encumbered for the instrument purchase. The acquisition is currently in progress, with the CSM Procurements working out the final terms and conditions and other contract language with the instrument provider (Scienta-Omicron). It is expected that the procurement process will be complete soon (within weeks), at which point we will begin working on the design drawings for the instrument. Payment will be made in installments over the course of 2017, with final payments made after acceptance of the instrument installation, expected in December, 2017.

Results Achieved

- As mentioned above, the instrument purchase is currently working its way through the procurement process at CSM.
- Laboratory space has been secured for the instrument in the new CoorsTek Center for Applied Science and Engineering, which will provide a highly visible, state-of-the-art home for the user facility and an avenue to publicize instrument capabilities and scientific output.
- The award has been leveraged for \$150,000 in additional funds to support add-on modules for the user facility to enable high-precision motorized control of sample

position, gas handling equipment for rapid variations in the chemical composition of the measurement environment, quadrupole mass analysis for in-line off-gas composition analysis (e.g. for TPD measurements coupled with the E-XPS measurements), and a glove-box load-lock for measurement of air-sensitive samples (such as battery equipment). These add-on modules will help make for a robust and powerful user facility for the characterization of next-generation materials.

 Negotiations with the instrument manufacturer have established working relationships and secured an opportunity for the center PIs/co-PIs to perform instrument verification tests at the company's headquarters in Germany. These experiments will help verify that the instrument capabilities best suit those of our user base, but will also provide exciting early data sets that we can use to promote and publicize instrument capabilities to attract a sizable instrument user base.

Summary of Benefits to the State of Colorado

- Received \$576,540 NSF core funds in 2016, to support instrument acquisition.
- The resulting user facility will leverage existing synergies in research capabilities and interest across numerous Colorado institutions CSM, NREL, NIST, UC Boulder, Colorado State University, and UCCS among them to enable ground-breaking materials science advances and enhance the reputation of Colorado acadmic and research institutions. The NSF proposal included letters of support from researchers at each of the aforementioned institutions, plus two Rocky Mountain institutions external to Colorado.
- The user facility also establishes a joint applications and development relationship between CSM and Scienta-Omicron, wherein the facility will be used for publicity purposes and also to develop new E-XPS environments and techniques to advance the state-of-the-art.
- The E-XPS facility will fill the gap in surface analysis education and will be utilized to advance students' knowledge of instrumentation, instrument capabilities, sample preparation, and data analysis relevant to their respective fields of study. We also envision wide exposure and hands-on experience to large population of students through other courses across the campus including but not limited to graduate course "Synthesis and Characterization of Solid State Materials" (co-PI Agarwal), and the undergraduate courses "Instrumental Analysis" (Y. Yang), "Materials Characterization and Instrumentation," "Surface Chemistry," and various topical colloquia offered across the campus.
- The PIs will also use the facility to improve secondary education in the Rocky Mountain region and nationally. In January of 2016, CSM graduate students, under mentorship of PIs Pylypenko and DeCaluwe are establishing an AVS student chapter. The chapter will organize demonstrations of vacuum technologies and tutorials on surface analysis for K-12, community colleges and several REU programs. Additionally, Rocky Mountain users *Pylypenko (CSM)* and *Christensen (UCCS)* organize and teach selected modules of Science Educators Workshop, a two day event which trains middle- and high-school science teachers to implement vacuum demonstrations and lesson plans in their own classrooms, held yearly during AVS International Symposium and Exhibition.
- The facility will promote student engagement in fundamental, applied, and interdisciplinary
 research in a university environment preparing them for research challenges of the real world.
 The presence of such a cutting-edge instrument on campus will expose graduate researchers on
 related projects to exciting research with transformative results that could alter the way they think

- about science. The facility will promote student participation at national and local conferences to present their research and initiate collaborations.
- In addition to promoting research activities of graduate students within various departments/programs, this facility will also promote research training of undergraduate students, for example those who receive CSM Undergraduate Research Fellowships or participate in REU programs conducted through the various campus research centers.

Publications in 2016 (funded wholly or in part with CHECRA funds):

Because the funds are all encumbered for purchase of an instrument which has not yet arrived, there are not yet any publications to report.