



March 1, 2016

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 2015.

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:

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; 2015 was the second year of funding.
2. The NSF had awarded a MRSEC grant to the Colorado School of Mines in 2008. CHECRA provided a cost share of \$400,000 for 6 years, with the final payment in 2014. In 2015, the School of Mines requested a supplemental 7th year of funding at fifty percent (\$200,000), to match a 7th year of "ramp-down" funding received from NSF. The School of Mines noted that the additional funding would enable Mines to pursue new opportunities to sustain the

Center. The Center is focused on investigating emerging renewable energy materials, such as the next generation of solar panels and fuel cells. It is the first NSF-funded center dedicated solely to renewable energy technologies. The CHECRA agreed to the request and provided a one-time supplemental payment of \$200,000 in 2015.

3. The Accelerating Innovation Research – Research Alliance (AIR-RA) project at Colorado State University, 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 first of three payments of \$136,000 toward this project.
4. The Center for Multiscale Modeling of Atmospheric Processes (CMMAP) at Colorado State University received its final of five payments of \$150,000 in 2015. CMMAP, which has received continued funding from NSF, is a partnership of research and educational institutions, government agencies, and industry aimed at developing a new kind of global atmospheric model. In addition to research, the Center has focused on educating and training a diverse population (specifically women, underrepresented minorities, and individuals with disabilities) in climate and Earth System Science; and knowledge transfer through the sharing of information with other modeling centers and the Colorado Governor's Energy Office.
5. The University of Colorado, the Colorado School of Mines and Colorado State University are 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 is providing a very limited cost share of 200,000 per year for 5 years, beginning in 2015.
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 fourth 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 Colorado School of Mines Re-inventing the Nation's Urban Water Infrastructure (ReNEWIt) Engineering Research Center received its final payment of \$400,000 from the Authority in 2015. With this grant from the NSF, the School of Mines joins leading universities in tackling the acute water problems and needed infrastructure changes facing the West.
8. The CHECRA provided cost shares for a number of 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 Northern Colorado: a single crystal x-ray diffractometer / \$93,783

University of Northern Colorado: a high performance computing cluster for multidisciplinary research and education / \$59,978

Colorado School of Mines: coupled optical and scanning microscopy facility / 64,858

University of Colorado Boulder: Shared Supercomputer by the Rocky Mountain Advanced Computing Consortium / \$140,000

University of Colorado Boulder: Infrared scanning near-field optical microscope (IR s-SNOM) for broadband nano-imaging and –spectroscopy / \$80,000

Colorado State University: Combined Spinning Disc Confocal/Atomic Force Microscopy System / \$95,000

Colorado State University: Ship-based C-Band Polarimetric Radar / \$125,000

Attachments to this report (Attachments B- XXXX) include detailed information on each of these projects. 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, all of 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] Symposium brings together hundreds of students, researchers, and professionals from universities, national laboratories and industry to exchange ideas and best practices in all areas of cyberinfrastructure.
- CMMAP [at CSU] reached over 20,000 K-12 students and teachers through the activities of the Little Shop of Physics (LSOP) in more than 40 school visits, science workshops and the LSOP annual open house.
- ... Through our summer teacher training workshops for K-12 teachers in Adams County and Denver Public Schools the [School of Mines] REMRSEC trained over 30 teachers to become proficient in delivering lessons on renewable energy topics that fit the state-mandated curriculum and are age appropriate for a specific grade. The Center also hosted 20 dyslexic students from grades 3-6 to enhance their proficiency in science and engineering concepts.
- ...the REMRSEC ran a research experiences for undergraduates program that provided quality research experiences for 24 undergraduate students from around the country. This program is an excellent recruiting tool to attract the best and the brightest future scientist and engineers to finish their educations in Colorado and hopefully remain here to bolster the scientific workforce.
- Because UNC is a comprehensive institution of higher education, integrating modern instrumentation into research and learning opportunities is highly valued. The single-crystal X-ray diffractometer will be central to the development of several courses that

address a variety of students to maximize the impact of the instrument. The XRD will provide research and educational experiences for undergraduates, graduate students, postdoctoral fellows, and high school teachers and students, many of whom will be trained to gain hands-on experience with crystallography.

- The [CU Center] conducted Family Science Evenings in partnership with a local Boulder community center and Arrupe Jesuit High School, a Denver urban high school that serves economically disadvantaged families...To date, four programs have been conducted at Red Oak serving 75 individuals, many of who are repeat attendees. At Arrupe High School in 2015 we conducted 2 evening programs and had a tremendous turnout in attendance from the Arrupe families. In a school with a student population of 350 there were more than 150 participants at each event

During calendar year 2015, the Authority received a single distribution of Limited Gaming Funds of \$2.1 million. Interest earnings on those funds totaled \$18,430, for a total income of \$2,118,430 in 2015. Payments to institutions are shown in the table in Appendix A. Total expenses were \$2,123,969.

Please contact me if you have any questions.

Sincerely yours,



Lt. Gov. Joseph A. Garcia
Chair

Attachments: Appendix A: CHECRA Expenses
Appendix B: University of Colorado MRSEC
Appendix C: School of Mines Renewable Energy MRSEC
Appendix D: Colorado State University AIR-RA
Appendix E: Colorado State University CMMAP
Appendix F: Colorado School of Mines Water Quality and Supply
Appendix G: Colorado School of Mines School of Mines Reinventing the
Nation's Urban Water Infrastructure
Appendix H: MRI Awards

Appendix A: CHECRA Expenses 2015

	Disbursements	Obligations*	
Colorado State University			
NSF Center for Multiscale Modeling of Atmospheric Processes (CMMAP)	150,000		
AIR-RA program	136,000		
MRI: Ship-based C-Band Polarimetric Radar		125,000	
MRI: Combined Spinning Disc Confocal/Atomic Force Microscopy System		95,000	
Colorado School of Mines			
Renewable Energy Materials Research Science and Engineering Center	200,000		
Engineering Research Center - Reinventing America's Urban Water Infrastructure	400,000		
NSF WSC Category 2 Collaborative	75,000		
Institute for Advanced Composites Manufacturing Innovation	100,000		
MRI: Coupled Optical and Scanning Microscopy Facility		64,858	
University of Colorado - Boulder			
Soft Materials MRSEC		400,000	
MRI: Shared Supercomputer		140,000	
MRI: Infrared scanning near-field optical microscope		80,000	
University of Northern Colorado			
MRI: Acquisition of a Single Crystal X-Ray Diffractometer	93,783		
MRI: Acquisition of a High Performance Computing Cluster	59,978		
 Total Obligated and Disbursed to Institutions in 2015	 1,214,761	 904,858	
Other Expenses	4,350		
Total Obligated and Disbursed	\$1,219,111	\$904,858	\$2,123,969

**due to processing delays, these payments were disbursed in 2016*

APPENDIX B: University of Colorado Soft Materials Research Center

NSF Grant DMR-1420736 (Previously DMR-0820579) to the University of Colorado, Boulder

Total CHECRA Grant funding: \$400,000 (per year for 6 years)

PIs Noel A. Clark, David M. Walba, Christopher N. Bowman, Jennifer N. Cha

SUMMARY

The Soft Materials Research Center began on the University of Colorado, Boulder (UCB) campus in the early 1980s. Block funding from the NSF Division of Materials Research began in 1995 with the incorporation of the UCB Liquid Crystal Frontiers Interdisciplinary Research Group (LCF IRG) into the NSF *Materials Research Science and Engineering Centers* (MRSEC) Program, as a member of an elite national network of advanced materials research centers. MRSEC renewal grants in 1998, 2002, and 2008 have continued support for the LCF IRG through 2014. In 2013 the UCB Campus applied for and was awarded another 6-year renewal, starting in November 2014. This renewal continued the LCF IRG and added a second IRG, the Click Nucleic Acids IRG, effectively doubling the size of Center and its NSF support to \$12M for 6 years through 2020. The State of Colorado through CHECRA is providing \$400K/yr for 6 years.

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

A major theme of materials science in the 21st century is understanding and manipulating the collective behavior and self-organization of complex molecules in soft materials and the expression of this organization at nanometer to macroscopic length scales. Within this context the SMRC focuses on the discovery of new materials phenomena and new materials paradigms. SMRC research is organized into two Interdisciplinary Research Groups, the *LIQUID CRYSTAL FRONTIERS* (LCF) IRG, and the *CLICK NUCLEIC ACIDS* (CNA) IRG. Each IRG melds synthesis, modeling, and physical studies into an intrinsically coherent synergistic effort, evolved into a collaborative research program in which the whole is greater than the sum of the parts. The progress to date has been achieved by making every effort to maintain seamless working relationships between the chemistry, physics, and engineering activities. The research proposed will enable us to exploit opportunities that have identified and, more importantly, expand the horizons and application of soft materials science in exciting new ways.

LIQUID CRYSTAL FRONTIERS (LCF IRG) - The LCF IRG 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 LCF IRG addresses 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.

CLICK NUCLEIC ACIDS IRG (CNA IRG) – The remarkable evolved capability of NAs for *sequence-directed self assembly (SDSA)* has been increasingly applied to the production of molecular architectures with rational and programmable control over shape, size, and function, leading in recent years to breathtaking advances in frontier nanoscale and bio sciences. While such proof-of-concept achievements promise dramatic new NA-based technologies, the realization of this potential faces key roadblocks:

•Firstly, NAs are expensive to synthesize in quantity. For example, at the current \$10K/gram they are prohibitively expensive even for high value-added technologies requiring gram quantities of material such as NA-based hydrogels for tissue regeneration, not to mention lower-value materials applications. •Secondly, neither the DNA backbone nor the DNA bases can be efficiently modified with the kind of elaborations of varying chemical functionality that have become important in polymer science. Even simple variations like changing the NA solubility profile or improving enzymatic or thermal stability is difficult. Realizing the potential of NAs, especially in the materials realm, will require dramatically lower cost, enhanced scalability, and a greatly expanded molecular structural scope.

The CNA IRG is organized to carry out a broad exploration of the SDSA of functional materials using Click Nucleic Acids (CNAs). CNAs are a novel DNA analog system, invented at UCB, in which oligomer chains with DNA-style sequences of selected bases are synthesized using thiolene click chemistry. The resulting thio-ether backbone/base structure is similar in its essential geometry to that of DNA and other NA analogs such as peptide nucleic acid (PNA), enabling CNA to exhibit sequence directed duplexing analogous to that of DNA. The rationale for CNA IRG research is our realization that the synergistic combination of click chemistry and oligo-nucleotide synthesis has dramatic advantages in expanding SDSA into the realm of practical materials science & technology. Specifically, photoinitiated thiol-X (-ene & -Michael) click chemistries provide robustness: **•stoichiometric reactant use; •rapid orthogonal reactions to completion; •minimal side reactions; •spatial and temporal reaction control; and •practical formation of higher molecular weight strands.** Monomer structural variations enabled with CNAs transform the native NA ACGTU alphabet of H-bonding side groups into a **multidimensional structural space** (MSS) wherein each monomer presents four distinct controllable elements: two independently controllable reactive functional end group linkers, a backbone segment, and a side group (generalized nucleobase). This MSS introduces powerful SDSA features not achievable with either DNA, RNA or other synthetic oligonucleotides such as PNAs. Thus, CNA monomers will have the capacity for structural variation of backbone features known to be critical in controlling the behavior of NAs, such as charge, chirality, solubility in organic or other solvents, stiffness, and electron transport. Variation of the end groups in the context of thiol-X click chemistry promotes facile ligation with other compounds on either end of sequences. Photoinitiation of thiol-X ligation enables photopatterning of sequence arrays with high yield. Finally, the use of click chemistry enables single pot synthesis of controlled sequence polymers in volume (3D) rather than on a surface (2D) as used for both DNA and PNA synthesis. The resulting materials scalability will dramatically lower the cost of oligomeric CNA, by 3 to 4 orders of magnitude relative to NAs or NA analogs. Efforts to date have successfully achieved: **•synthesis of CNA homopolymers; •synthesis of sequence specific CNA oligomers; •measurement of binding constants for CNA-CNA and DNA-DNA hybridization** (CNA exhibits stronger and more selective base pairing than DNA); **•modeling and visualization of CNA hybridization using atomistic MD simulation; •volume batch preparation of monomers and polymers.**

With this vision, the CNA-IRG team, a highly interactive and coherent collaboration with expertise ranging from thiol-ene click photochemistry and atomistic computer simulation, to soft-matter nanophotonics and bioscience, will pursue the opportunities presented by CNA with a two-pronged approach: **•CNA molecular design, modeling, synthesis, & characterization and •exploration of CNA SDSA functionalities in a variety of interfacial and bulk, near-term and high-risk, materials and bio realm applications.** The design and synthesis thrust will focus on developing highly scalable synthetic processes for CNAs, on exploring the MSS by expanding the nucleobase alphabets and controlling the backbone and side chains to tailor molecular compatibility. The self-assembly thrust takes advantage of the enhanced programmability and design flexibility afforded by CNAs, in applications of SDSA, including polymer materials development, nanotemplating, block copolymers, and hydrogels.

FUNDING ALLOCATED TO EACH PRINCIPAL PERSON OR ENTITY

In 2015 the CHECRA funding was allocated to the three focus areas of the Center described in this summary – research, industrial & National Laboratory outreach, and education outreach.

Research - The past year of MRSEC, with NSF funding supplemented by the CHECRA matching state funds, has continued in its role as UCBs single most visible materials research group nationally and internationally. Major research accomplishments are as follows:

Heliconical Nematic Phase - Observation of heliconical nematic ordering in a liquid crystal made from bent molecular dimers has enabled the discovery of the first new nematic phase in over 50 years. The LCF IRG has led the way in visualizing the heliconical ordering and measuring its helical pitch using freeze-fracture transmission electron microscopy and resonant x-ray scattering, both techniques that the SMRC pioneered in the study of liquid crystals. The HN phase promises a host of new liquid crystal applications in chemical synthesis of chiral materials such as pharmaceuticals and in chiral separations.

Room Temperature Ionic LCs - RTILs are low melting-temperature, organic salts, of great utility because of near-zero vapor pressure, fully tailorable solubility, high polarity, and non-coordinating nature. The Center is leading in the development of photopolymerized nanoporous materials having RTIL nanochannels. Such RTIL liquid crystal systems will be pursued in the development of the polymerization of biphilic lyotropic nanoporous media for electrolytes and separations.

Click Nucleic Acids – 2015 saw the first major research benchmark of the CNA IRG, with it publication of the success of their proposed click chemistry for making DNA homologs in the world leading chemistry journal Angewandte Chemie:

“CLICKABLE NUCLEIC ACIDS: SEQUENCE-CONTROLLED PERIODIC COPOLYMER/ OLIGOMER SYNTHESIS BY ORTHOGONAL THIOL-X REACTIONS,”
W. Xi, S. Pattanayak, C. Wang, B. Fairbanks, T. Gong, J. Wagner, C.J. Kloxin, and C.N. Bowman, Angewandte Chemie International Edition, **54**, 1 – 7 (2015).

Industrial & National Laboratory Outreach – Liquid Crystal Frontiers – In collaboration with Lawrence Berkeley National Laboratory we have developed resonant x-ray scattering as an effective probe of liquid crystal structure, enabling the discovery of the heliconical nematic phase, discussed above.

The Center has been a major innovator in the field of ferroelectric liquid crystals (FLCs) for many years. Displaytech, Inc., a Colorado company founded by the Center PI and Co-PI, has successfully commercialized FLC in the form of microdisplays for camera viewfinders and hand-held picoprojectors. The Displaytech team continues to manufacture liquid crystals for its display products in Longmont.

Click Nucleic Acids – The SMRC has spun-off the start-up company Click Nucleic Acids, Inc. a Colorado company, formed to commercialize novel nucleic acid synthesis technology under license from UCB. Initial products will focus on the biotechnical applications of CNAs in gene sequencing and tissue generation.

Education Outreach, Diversity - The SMRC conducted Family Science Evenings in partnership with a local Boulder community center and Arrupe Jesuit High School, a Denver urban high school that serves economically disadvantaged families. Family Science Evening enables students and their parents to experience and explore science and engineering together. Center faculty, who give an introduction to an interactive science topic and activities, lead the evening program. Graduate and undergraduate students engage and assist the families with the small group, table-top activities.

This program supports: (i) education and empowerment of parents so that they can better further their children’s education; (ii) encouragement of the participation of underrepresented minorities in Science, Technology, Engineering, Mathematics (STEM) education; (iii) development of program content with appropriate pedagogical strategies focusing on the engineering design process and the scientific methodology, while producing engaging sessions that help young children and their families develop science and engineering skills and knowledge.

Since its inception in Fall 2013, six Family Science Evenings have been conducted. The Boulder programs are held at the Red Oak Community Center. This Center serves a local community of underrepresented minorities and economical disadvantaged families. To date, four programs have been

conducted at Red Oak serving 75 individuals, many of who are repeat attendees. At Arrupe High School in 2015 we conducted 2 evening programs and had a tremendous turnout in attendance from the Arrupe families. In a school with a student population of 350 there were more than 150 participants at each event.

Renewable Energy Materials Research Science and Engineering Center
Colorado School of Mines
CHECRA Grant: \$400,000 (per year for 6 years); \$200,000 for one year

Summary: The Materials Research Science and Engineering Center (MRSEC) at the School of Mines, under the leadership of Dr. Craig Taylor, is focused on investigating emerging renewable energy materials, such as enhancing solar panels through nanotechnology and improving membrane technologies important to renewable energy applications, such as batteries, fuel cells and electrolyzers.

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

With annual global energy consumption expected to increase to as much as 30 terawatts by 2050 and mounting concerns over oil reserve depletion, energy security, and global warming, meeting world energy demand will be one of the grand challenges of the 21st century. While renewable and alternative technologies have the potential to address the most serious concerns with fossil fuels, cost is a major obstacle to their widespread deployment. There has been remarkable progress, for example, in lowering the price of photovoltaic (PV) electricity generation, yet present costs remain higher than electricity produced from coal. Similar price differentials exist when comparing fuel cells with conventional electricity generators. Estimates based on historical trends give several decades before many renewable technologies become competitive. Transformative technological innovation is the key to accelerating this time line and fundamental advances in materials science will spearhead this process.

The MRSEC consists of two Interdisciplinary Research Groups (IRGs). IRG1 has concentrated on materials of potential use in the next generation of PV devices, but the scope of this IRG is much broader since the systems of interest have important properties in common with a wide range of other electronic and opto-electronic materials. The important questions this IRG has attempted to answer involve the scattering and relaxation mechanisms that govern electronic transport in semiconducting materials of use in PV applications, especially mechanisms that are altered in nanostructured environments. These nanostructures include quantum wires and quantum dots, which have potential for significant improvements in efficiency by tuning the optical and electronic properties through size, composition, and surface termination, and by uniquely quantum mechanical effects, which offer possibilities for collecting solar radiation that is lost in conventional cells. The long-term research directions of this IRG were aimed at producing transformative changes in PV technology through significant improvements in materials properties that result from development of fundamental concepts for more efficient carrier generation and collection. This IRG completed its work in 2015 and has been shut down.

The second Group (IRG2) has concentrated on advanced membranes for renewable energy applications, with the scope being also much broader since the systems to be studied include polymers, ionic solids, and hybrid systems. Solid electrolyte materials and membrane technologies are central to many processes in the conversion, utilization, and storage of energy. Very frequently, ionic transport is the "weak link" in electrochemical energy storage or conversion systems. At present, the myriad interactions that occur in ion transport

Appendix C: Colorado School of Mines, Materials Research Science and Engineering Center in Renewable Energy

membranes- ion-ion, ion-solvent, and ion-electrode-are poorly understood. Fundamental research is crucially needed to provide the knowledge required for the intelligent design of novel transport membranes with highly optimized properties. IRG2 has fabricated novel transformative ion conducting materials by synergistically combining materials with dramatically different ionic transport characteristics. This IRG completed its work in 2015 and has been shut down.

An additional research group involves the evaluation of clathrate structures as potential materials for renewable energy applications, such as hydrogen storage, photovoltaics, and membranes for ionic transport. Energy storage, and in particular storage of hydrogen or methane produced from renewable resources, is another area of research in renewable energy where transformative research is critical. Clathrate hydrates, with as much as 164 volumes of gas contained per volume of clathrate hydrate, present a potentially attractive class of energy storage compounds. Center scientists and engineers have succeeded in making silicon clathrate materials in larger volumes for our experiments in using these materials in solar cells. Recently, thin films of clathrate silicon have been produced. This accomplishment is significant because thin films are necessary in order to use these materials in solar cells.

1. In addition to the two research groups, funds were used to support "seed" grants on promising but very preliminary research projects. Five projects funded in 2015 were entitled:

Exotic Forms of Silicon for the Next Generation Electronic and Photonic Materials

Carolyn Koh, Mark Maupin, Reuben Collins, Lakshmi Krishna, Chip Durfee, Paul Stradins (NREL), Timothy Strobel (Carnegie Institution)

2. Harnessing the Order Parameter in Optoelectronic Semiconductors

Eric Toberer, Jeff Squier, Jeremy Zimmerman, Vladan Stevanovic, Lakshmi Krishna, Adele Tamboli (NREL), Andriy Zakutayev (NREL)

3. The Materials Genome Gets Hot: Integrating Theory and Experiment to Incorporate Finite Temperature Effects into Modern Materials by Design

Vladan Stevanović, Ryan O'Hayre, Jianhua Tong, Anriy Zakutayev

4. Bringing new compositions of matter to life: Computationally guided synthetic approaches to unprecedented nanoscale metal carbide/nitride materials

Ryan Richards, Christian Ciobanu, Svitlana Pylypenko, Brian Trewyn

5. Novel Metal Organic Framework (MOF) Membranes and Microporous Carbon Membranes Derived from MOF for Natural Gas Purification

Moises A. Carreon, Brian G. Trewyn, Alan Sellinger

Principal Senior Investigators

Funding from CHECRA

P. Craig Taylor, Director

\$20,000

Reuben Collins, Associate Director and Head

\$60,000

IRG 1

Andrew Herring, Head IRG2

\$60,000

Carolyn Koh, Head, Seed Grant Program and Head

\$60,000

IRG3

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

P. Craig Taylor: Discretionary funding of promising new research directions.

Reuben Collins: Funding for films of silicon nanodots imbedded in an amorphous silicon matrix for improved solar cell materials

Andrew Herring: Funding for organic-inorganic nanostructured membranes for fuel cell and battery applications

Carolyn Koh: Funding of novel approaches to new materials for photovoltaic applications or membrane technologies. Funding for development of clathrate materials for renewable energy applications.

Results achieved

1. Exotic Forms of Silicon for the Next Generation Electronic and Photonic Materials

The vision is to discover, design and explore the fundamental materials science of revolutionary new electronic and optoelectronic silicon-based materials. The aim is to uncover how structures can be controlled to exhibit unique properties not possible in conventional forms of Si. Success will uncover how structure and dimensionality control optoelectronic characteristics, while simultaneously developing the next generation of Si-based materials for high performance and low cost applications. We are realizing this vision through fundamental innovative research directed at exotic forms of Si (e.g. new Si allotropes, chalcogenides). Strongly coupled computation and novel synthesis and characterization methods are being developed and applied at ambient and extreme P, T conditions. An integrating focus is materials to revolutionize solar devices, which represents a *Grand Challenge*.

2. Harnessing the Order Parameter in Optoelectronic Semiconductors

Advances in optoelectronic technologies have historically stemmed from isoelectronic alloying of III-V materials to tune properties such as band gap, absorption/emission strength, refractive indices, and lattice parameter. However, these properties are fundamentally linked, resulting in a narrow set of material properties that can be practically integrated through epitaxial growth due to constraints on lattice matching. These limitations have resulted in the need for extraordinary measures to fabricate advanced structures, such as thick metamorphic grade layers to access multiple band gaps in multi-junction solar cells. Over the last year, our team has begun to address this grand materials challenge. Our efforts revealed the order parameter in ternary diamond-like semiconductors provides incredible control of optoelectronic properties without changing the lattice constant significantly. One example of order parameter control is in the II-IV-V₂ materials, a class of compounds similar to III-Vs, but with a doubled unit cell size due to the substitution of group II and IV elements for group III cations. Tuning the order parameter can result in about 1 eV of band gap tunability. This effect is significantly larger than the similar phenomenon of isoelectronic cation ordering in ternary III-V materials such as GaInP₂. The remaining questions are:

- _ How are band structure and character of band edges affected by the order parameter?
- _ How do optical transition probabilities evolve with disorder?
- _ What is the impact of disorder on carrier localization and minority carrier lifetime?
- _ What is the role of cation clustering on these properties?

3. The Materials Genome Gets Hot: Integrating Theory and Experiment to Incorporate Finite Temperature Effects into Modern Materials by Design

Enabled by the rapid increase in computing power, significant method advances, and the tightening integration of computation with experiment, materials by design is rapidly becoming a leading paradigm in materials science. The true potential of this approach to accelerate the pace of materials design and discovery has been recognized by the Materials Genome and related initiatives. However, for their potential to be fully realized, materials by design and associated approaches need to overcome the important discontinuities between computation on one side and experiment on the other. Our vision is to bring first principles theory closer to the experimental reality by taking into account finite temperature effects, which are essential for describing the behavior of materials at their typical operating and/or growth conditions. Finite temperature effects encompass both enthalpy and entropy contributions to the free energy of solids as well as the effects of disorder, both atomic and magnetic, on physical properties. Presently, these effects are treated on a case-by-case basis and are not usually taken into account in broad material searches. Neglecting entropy and finite temperature contributions to the enthalpy of solid phases can lead to serious inaccuracies in predicting stability. Similarly, neglecting disorder can lead to inaccurate predictions of materials properties. For example, the electronic structure of a PV material $\text{Cu}_2\text{ZnSnSe}_4$ is known to be very sensitive of the state of cation disorder as well as electrical transport in spinel oxides. Our preliminary calculations have confirmed this result.

4. Bringing new compositions of matter to life: Computationally guided synthetic approaches to unprecedented nanoscale metal carbide/nitride materials

Interest in metal carbides and nitrides originates from a 1973 *Science* paper concluding that Group VI transition metals and carbon can result in materials with Pt-like properties with regard to activity, selectivity, and resistance to poisoning. Using valence bond theory, it was deduced that molybdenum and tungsten carbides/nitrides combine their valence *sp* electrons with metal *spd* bands resulting in structures with chemical reactivity that resembles that of noble metals. Early transition metal (groups III-VI) carbides/nitrides have been reported for several important processes: adsorption and activation of hydrogen, deoxygenation, and hydrodeoxygenation reactions, as well as hydrogen evolution for water splitting. These materials are typically derived utilizing high temperature reactions with carbon and nitrogen sources in the gas phase, using metal, metal oxide or metal salts as the starting material. However, these high temperature preparation routes generally do not offer control over the size and morphology. Such limitations are even more pronounced for the carbides/nitrides of later transition metals (VIII-X), which are more abundant and less expensive but largely unexplored. To identify materials structures with desirable properties, materials discovery and design may be assisted by high-throughput computational screening. Synthesis and characterization can then focus on the most promising materials. However, employing direct screening hinges on the assumption that the desired properties can be computed rapidly. When such rapid computation of properties is not possible, the current state-of-the-art relies on discovering approximate “predictor” properties, which can be computed easily and are largely correlated with the desired properties. Screening via such predictors is fast and leads to an improved set of materials that we have shown can then be experimentally tested. Furthermore, this approach is leading to intriguing connections between desired properties and their predictors.

5. Novel Metal Organic Framework (MOF) Membranes and Microporous Carbon Membranes Derived from MOF for Natural Gas Purification

Natural gas consists primarily of methane, higher alkanes, carbon dioxide, nitrogen, and hydrogen sulfide. In particular, CO_2 and N_2 decrease the heat value of natural gas. Therefore, it is highly desirable to remove CO_2 and N_2 from natural gas in order to improve its heat content. Approximately 14% of U.S. natural gas contains >4% nitrogen, and thus nitrogen rejection technologies are required. Most of the N_2 rejection plants use a cryogenic distillation process, which is very costly. To compete with cryogenic distillation, the great challenge of applying more

energy-efficient membrane separation technology is to develop membranes that effectively separate N_2/CH_4 mixtures. However, the current state-of-the-art N_2 -selective polymeric membranes display low N_2 permeabilities, and low separation selectivities. Recently, we have incorporated some inorganic materials into N_2 -selective membranes and shown N_2/CH_4 separation performances above the so-called “upper bound” observed for polymers. However, these membranes cannot provide sufficient selectivity and N_2 permeance to compete with conventional natural gas purification technologies. Therefore, there is a critical need to develop novel membranes with fundamentally different transport and adsorption properties than those of conventional materials (zeolites and polymers) that could reduce the costs associated with natural gas purification and leapfrog the current separation technologies.

We have developed novel metal organic framework (MOF) membrane compositions and microporous carbon membranes derived from MOFs with tunable pore sizes, and controlled surface functionalities for CO_2/CH_4 and N_2/CH_4 separation. Preliminary results show that the resultant membranes probably display unique adsorption properties (from acidic, neutral to basic) which are known to influence the separation selectivity toward different gas mixtures. In addition, these membranes may display a molecular sieving effect, due to the presence of micropores with sizes in the range of the molecular gases to be separated.

Publications in 2015:

Seed Funding-Partial CHECRA Support

- M. Duke, B. Zhu, C. Doherty, M. Hill, A. Hill, M. Carreon, “Structural effects on SAPO-34 and ZIF-8 materials exposed to seawater solutions, and their potential as desalination membranes”, *Desalination* 2016.
- S. Venna, M. Carreon, “Metal organic framework membranes for carbon dioxide separation”, *Chemical Engineering Science*, March 2015
- X. Feng, M. Carreon, “Kinetics of transformation on ZIF-67 crystals”, *Journal of Crystal Growth*, May 2015
- A. Nambo, C. Miralda, J. Jasinski, M. Carreon, “Methanolysis of Olive Oil for biodiesel synthesis over ZnO nanorods,” *Reaction Kinetics, Mechanisms and Catalysis*, 2015.
- C. Chen, X. Zhang, L. Krishna, C. Kendrick, S. Shang, E. Toberer, Z. Liu, A. Tamboli, J. Redwing, “Synthesis, characterization and chemical stability of silicon dichalcogenides, $Si(SexS_{1-x})_2$,” *Journal of Crystal Growth*, December 2015.
- L. Krishna, P. Chai, C. Koh, E. Toberer, G. Nolas, “Synthesis and structural properties of type I potassium SiGe alloy clathrates,” *Materials Letters*, June 2015.
- L. Krishna, C. Koh. “Inorganic and methane clathrates: Versatility of guest-host compounds for energy harvesting,” *MRS Energy and Sustainability*, 2015.

- A. Martinez, B. Ortiz, N. Johnson, L. Baranowski, L. Krishna, S. Choi, P. Dippo, B. To, A. Norman, P. Stradins, V. Stevanovic, E. Toberer, A. Tamboli. "Development of ZnSiP for Si-Based Tandem Solar Cells," *IEEE Journal of Photovoltaics*, January 2015.
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- A. Martinez, E. Warren, P. Gorai, K. Borup, D. Kuciauskas, P. Dippo, B. Ortiz, R. Macaluso, S. Nguyen, A. Greenaway, S. Boettcher, A. Norman, V. Stevanovic, E. Toberer, A. Tamboli. "Solar energy conversion properties and defect physics of ZnSiP₂", *Energy and Environmental Science*, December 2015.
- A. Fioretti, A. Zakutayev, H. Moutinho, C. Melamed, J. Perkins, A. Norman, M. Al-Jassim, E. Toberer, A. Tamboli, "Combinatorial insights into doping control and transport properties of zinc tin nitride," *Journal of Materials Chemistry*, September 2015.
- C. Duan, J. Tong, M. Shang, S. Nikodemski, M. Sanders, S. Ricote, A. Almonsoori, R. O'Hayre, "Readily Processed Protonic Ceramic Fuel Cells with High Performance at Low Temperatures", *Science*, July 2015.
- P. Joghee, J. Nekuda Malik, S. Pylypenko, R. O'Hayre, "A review on direct methanol fuel cells - in the perspective of energy and sustainability", *MRS Energy and Sustainability*, May 2015.
- A. Deml, A. Holder, R. O'Hayre, C. Musgrave, and V. Stevanović, "Intrinsic Material Properties Dictating Oxygen Vacancy Formation Energetics in Metal Oxides", *Journal of Physical Chemistry Letters*, May 2015.
- J. Fish, S. Ricote, R. O'Hayre, N. Bonanos, "Electrical properties and flux performance of composite ceramic hydrogen separation membranes", *Journal of Materials Chemistry*, January 2015.

Education and Outreach - Partial CHECRA Support

- none

In 2015 the REMRSEC supported over 30 postdoctoral research associates, graduate students, and undergraduate students. Through our summer teacher training workshops for K-12 teachers in Adams County and Denver Public Schools the REMRSEC trained over 30 teachers to become proficient in delivering lessons on renewable energy topics that fit the state-mandated curriculum and are age appropriate for a specific grade. The Center also hosted 20 dyslexic students from grades 3-6 to enhance their proficiency in science and engineering concepts. This is particularly

high aptitudes for mathematics and science subjects, but they often get left behind in a traditional learning environment. Finally, the REMRSEC ran a research experiences for undergraduates program that provided quality research experiences for 24 undergraduate students from around the country. This program is an excellent recruiting tool to attract the best and the brightest future scientist and engineers to finish their educations in Colorado and hopefully remain here to bolster the scientific workforce.

Appendix D: Advanced Thin Film Photovoltaics for Sustainable Energy

NSF AIR:RA Award
Colorado State University
CHECRA Grant (\$400K for 3 years)

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 Cd_{1-x}Mg_xTe 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:

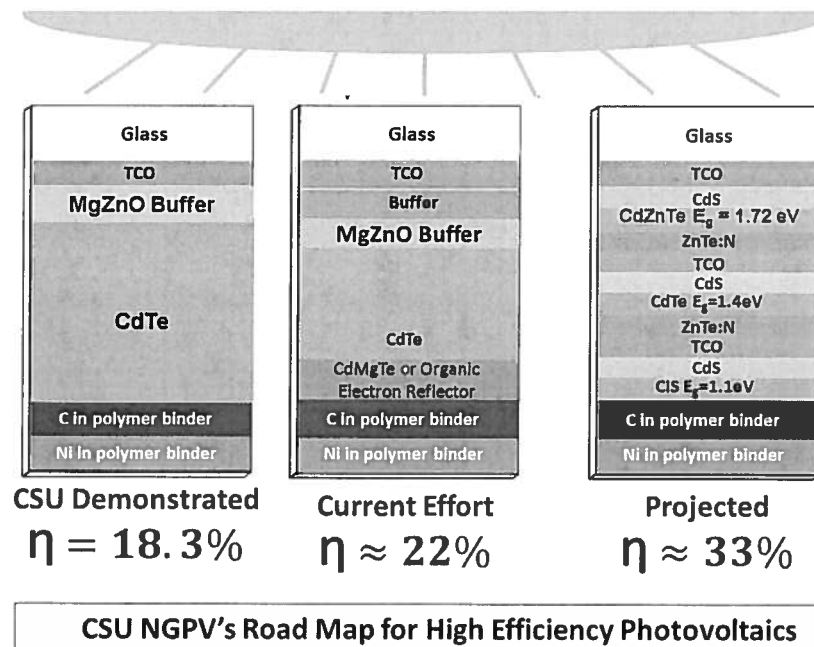


Figure 1: Efficiency Roadmap for CdTe Photovoltaics at CSU

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 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 and is currently being fabricated. 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. 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.

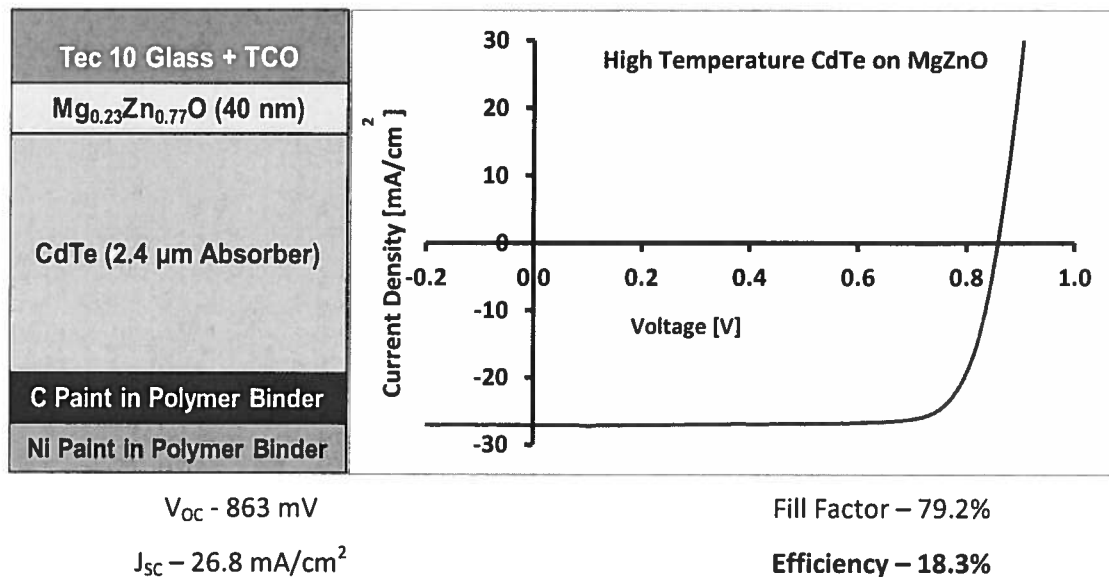


Figure 2: Device Structure for 18.3% efficiency device and the JV curve (J in mA/sq. cm. on the y-axis and volts on the x-axis).

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. Amit H. Munshi, Jason M. Kephart, Ali Abbas, John M. Walls and W.S. Sampath titled "Effect of Varying Deposition Source and Substrate Temperature on CSS CdTe Thin-film Photovoltaics" submitted to 43rd IEEE PVSC.
2. D. E. Swanson, J. M. Kephart, P. S. Kobayakov, 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. Carey Reich. Drew Swanson, Jennifer Drayton, Amit Munshi, Ali Abbas, Walajabad Sampath; "Development of Cd_{1-x}Mg_xTe Photovoltaics for use in a Tandem Cell", submitted to IEEE PVSC.

Appendix E: Center for Multiscale Modeling of Atmospheric Processes (CMMAP)

Colorado State University

Principal Investigators:

Center Director: David A. Randall, Colorado State University

Deputy Director: Chin-Hoh Moeng, The National Center for Atmospheric Research, Boulder, Colorado

Director for Education and Diversity: A. Scott Denning, Colorado State University

Director for Knowledge Transfer: Steve Krueger, University of Utah

Director for Cyberinfrastructure: John Helly, University of California, San Diego

Project Description

The Center for Multiscale Modeling of Atmospheric Processes (CMMAP) is one of seventeen current Science and Technology Centers (STCs) sponsored by the National Science Foundation. Up to this time, CMMAP is the only STC ever awarded in the state of Colorado. CMMAP is a partnership of research and educational institutions, government agencies, and industry.

CMMAP's activities are divided into three areas: (1) research, which is focused on developing a new kind of global atmospheric model; (2) education, outreach and diversity, which seeks to educate and train a diverse population (specifically women, underrepresented minorities, and individuals with disabilities) in climate and Earth System Science; and (3) knowledge transfer, through the sharing of information with other modeling centers and the Colorado Governor's Energy Office. CHECRA funding is being used to support all three of these focus areas.

The Center's research is focused on improving the representation of cloud processes in climate models. Cloud processes are central to the Earth Sciences. Changes in cloudiness can either amplify or damp climate change. In addition, cloudiness and precipitation are key elements of any weather forecast. Clouds are central components of the water cycle. Chemical transformations occur inside clouds and feed back to affect the properties of the clouds. Last but not least, the biosphere is highly dependent on cloud processes. Progress in all of these disciplines is being held back by our limited ability to understand and simulate global cloudiness.

CMMAP's vision is to take advantage of rapidly increasing computer speed to achieve major advances in our ability to understand and predict the effects of clouds on weather and climate, through a revolutionary new approach called the "multi-scale modeling framework" (MMF), in which high-resolution cloud models are coupled to lower-resolution global models. CMMAP's research team includes climate modelers, cloud modelers, and experts on turbulence, radiation, cloud physics, and observations.

CMMAP also has major activities in the areas of Education and Diversity. CMMAP's graduate students are immersed in the Center's culture. They see, and some of them participate in, the training of high-school science teachers and the teaching and mentoring of diverse undergraduates. The students work collaboratively with faculty, solving problems together.

Through “the Center experience,” these future leaders are gaining a broad and deep perspective on what it means to be a scientist. In years to come, the larger U.S. society will benefit from this.

The Center’s research, education, and diversity missions have the potential to feedback positively on each other. Through its outreach and education work, CMMAP has built credibility with diverse communities. This credibility invites those communities to consider how CMMAP’s science mission can serve their priorities. CMMAP’s experience in knowledge transfer provides strategies for moving from the basic research to practical knowledge that the communities can use. Finally, the broad experiences of CMMAP graduate students prepare them to link research, education, and diversity. This a positive feedback loop that enriches the research, attracts diverse communities and students, and transfers knowledge to users, all based on the connections that are forged within the Center.

How the CHECRA funding was used

The Center for Multiscale Modeling of Atmospheric Processes (CMMAP) at Colorado State University received the final of five payments of \$150,000 from the Authority in 2015. CMMAP is a partnership of research and educational institutions, government agencies and industry and it focuses its research on improving the representation of cloud processes in climate models.

The final year of CHECRA funds was used to support one administrative professional and two research scientists at Colorado State University. The administrative personnel provide essential operational support for CMMAP, including financial management and the organization of a broad range of research and educational activities. The two research scientists who are receiving partial salary support from CHECRA are Ross Heikes and Celal Konor. They are developing new mathematical methods to represent weather and climate processes, and doing theoretical work on the role of water vapor in the tropical atmosphere. CHECRA funding was also used to support travel for visiting scientists.

In addition, some of the CHECRA funds were used to support components of a computer cluster including two RAIDs (Redundant Array of Inexpensive Disks) which serves as an expansion of disk storage for extensive cloud modeling data as well as computer modeling workstations. The Science and Technology Center requires high capacity workstations for data collection, processing, and model integrations. CMMAP’s super parameterizations cloud modeling projects involve exclusive model output that is highly specialized and intended primarily for analysis by the project team.

Summary of Benefits to the State of Colorado

- CMMAP was renewed by the National Science Foundation through June 2016, through an award of \$17,991,000 to Colorado State University, much of which is used to pay the salaries of staff and graduate students who live in Colorado.
- CMMAP reached over 20,000 K-12 students and teachers through the activities of the Little Shop of Physics (LSOP) in more than 40 school visits, science workshops and the LSOP annual open house.

- CMMAP provided an intensive week long training to 45 teachers, elementary through high school with the Teaching Weather and Climate Summer Teacher Course.
- CMMAP supported the Windows to the Universe website, which had 6,158,872 page views from 4,050,930 visitors.
- CMMAP supported 16 CSU graduate students and 9 undergraduate summer interns. Several of these interns are expected to attend graduate school at CSU.
- CMMAP has hosted team meetings in Fort Collins annually bringing about 40 visitors per year to Colorado.
- CMMAP supported the 2015 LSOP Weather and Science Day which was held at Coors Field in Denver, CO on April 23, 2015. This educational event provides an interactive presentation that incorporates physics, math, and meteorology into unique science experiments and reaches an audience of ~15,000 middle and high school students.

Journal Publications for 2015

1. Thayer-Calder, K., and D. A. Randall, 2015: Examining Boundary Layer Quasi-Equilibrium with Cloud Model Simulations. *Geophys. Res. Lett.*, **42**, doi:10.1002/2014GL062649.
2. Firl, G., and D. A. Randall, 2015: Fitting and Analyzing Large-Eddy Simulations Using Multiple Trivariate Gaussians. *J. Atmos. Sci.*, **72**, 1094-1116. doi: <http://dx.doi.org/10.1175/JAS-D-14-0192.1>.
3. Arnold, N. P., M. Branson, Z. Kuang, D. A. Randall, and E. Tziperman, 2015: MJO intensification with warming in the super-parameterized CESM. *J. Climate*, **28**, 2706-2724. doi: <http://dx.doi.org/10.1175/JCLI-D-14-00494.1>
4. Arnold, N. P., and D. A. Randall, 2015: Global-scale convective aggregation: Implications for the MJO. *J. Adv. Modeling Earth Syst.*, **7**, doi:10.1002/2015MS000498.
5. Jiang, X., D. E. Waliser, P. K. Xavier, J. Petch, N. P. Klingaman, S. J. Woolnough, B. Guan, G. Bellon, T. Crueger, C. DeMott, C. Hannay, H. Lin, W. Hu, D. Kim, C. -L. Lappen, M. -M. Lu, H. -Y. Ma, T. Miyakawa, J. A. Ridout, S. D. Schubert, J. Sinocca, K. -H. Seo, E. Shindo, X. Song, C. Stan, W. -L. Tseng, W. Wang, T. Wu, X. Wu, K. Wyser, G. J. Zhang, and H. Zu, 2015: Vertical structure and physical processes of the Madden-Julian Oscillation: Exploring key model physics in climate simulations. *J. Geophys. Res.*, doi:10.1002/2014JD022375.
6. Krishnamurthy, V., and C. Stan, 2015: Simulation of the South American climate by a coupled model with super-parameterized convection. *Clim. Dyn.*, doi:10.1007/s00382-015-2476-6.
7. Randall, D. A., A. D. Del Genio, L. J. Donner, W. D. Collins, and W. A. Klein, 2015: The Impact of ARM on Climate Modeling. *The Atmospheric Radiation Measurement Program*:

The First 20 Years, D. D. Turner and R. Ellingson, Eds., which will be published as a *Meteorological Monograph* by the American Meteorological Society. In press.

8. Randall, D. A., C. DeMott, C. Stan, M. Khairoutdinov, J. Benedict, R. McCrary, and K. Thayer-Calder, 2015: Simulations of the tropical general circulation with a multiscale global model. *Yanai Memorial Volume*, a *Meteorological Monograph* published by the American Meteorological Society. In press.
9. Burt, M. A., D. A. Randall, and M. D. Branson, 2015: Dark warming. *J. Climate*. In press.
10. Kooperman, G. J., M. S. Pritchard, M. A. Burt, M. D. Branson, and D. A. Randall, 2016: Robust effects of cloud super-parameterization on simulated daily rainfall intensity statistics across multiple versions of the Community Earth System Model. Submitted to *J. Adv. Modeling Earth Syst.*

Appendix F: School of Mines, Water Quality and Supply Impacts from Climate-Induced Insect Tree Mortality

Integrated GroundWater Modeling Center (IGWMC)

Colorado School of Mines

CHECRA Grant: \$75,000 (per year for 5 years)

Reporting Period: January 1-December 31, 2015

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

Appendix F: School of Mines, Water Quality and Supply Impacts from Climate-Induced Insect Tree Mortality

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	\$40,680
Jonathan Sharp	\$0
John McCray	\$40,043
Alexis Navarre-Sitchler	\$0
Total Spending (Jan. – Dec. 2015)	\$80,723

Students and Postdocs (* funded through CHECRA)

Name	Affiliation	Research
Lindsay Bearup	CSM postdoctoral research fellow	Hydrological effects of forest transpiration loss in bark beetle-impacted watersheds
Kristin Mikkelsen	CSM postdoctoral research fellow	Bark beetle infestation impacts on nutrient cycling, water quality and interdependent hydrological effects
Jennifer Jefferson	CSM graduate student	Modeling an idealized domain with homogeneous forest land cover and a heterogeneous subsurface representation of a Rocky Mountain watershed
Elanor Heil	CSM graduate student	Metal cycling in Mountain Pine Beetle impacted watersheds
Chelsea Bokman	CSM graduate student	Soil microbial nutrient cycling and impacts on carbon and nitrogen outputs
Brent Brouillard	CSM graduate student	Drinking water quality impacts
Nicolas Jeangros Rodriguez*	CSM graduate student	Modeling future impacts of forest insect infestations on the carbon cycle in streams and groundwater
Mary Michael Forrester	CSM graduate student	Modeling groundwater age resulting from transpiration loss in beetle-infested areas
Nicole Bogenschuetz*	CSM graduate student	Field characterization of soil mineralization
Mike Morse	CSM graduate student	Education and outreach
Lisa Gallagher	CSM research associate	Education and outreach

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

Reed Maxwell: Partial tuition and stipend support for one graduate student at CSM: Nicole Bogenschuetz (MS student, HSE). Nicole is studying the effect of the Mountain Pine Beetle on stability, soil moisture distribution, and root strength on beetle-infected mountain slopes. Partial summer salary was also provided to Prof Maxwell who is supervising students Jefferson, Forrester,

Appendix F: School of Mines, Water Quality and Supply Impacts from Climate-Induced Insect Tree Mortality

and Bogenschuetz and supervising Dr. Bearup, Dr. Gallagher, and Morse.

John McCray: Dr. McCray is supervising and giving partial tuition and stipend support to graduate student Nicolas Rodriguez, who is working on modeling the future impacts of forest insect infestations on the carbon cycle in streams and groundwater.

(c) The results achieved by the project

Nicole Bogenschuetz explored the effects of MPB infestation on slope stability. The roots cease to transpire three to four years proceeding infestation; therefore, root tensile strength decreases. This was investigated through in-situ tensile strength measurements. However, this effect on the hillslope is likely counteracted by the regrowth of grasses, forbs, shrubs, and trees. In addition, the rise of the water table, from the lack of transpiring trees, is adding a driving force to the slopes. The fluctuation in the water table is being modeled using an integrated hydrologic model (ParFlow) on a theoretical hillslope. The combination of the decrease in root tensile strength and fluctuations of the water table will be used to assess the impact of MPB tree mortality on slope stability through examining changes in the factor of safety. The factor of safety is being calculated using an infinite slope model. Preliminary results displayed a decrease in a factor of safety, particularly at the toe of the slope, which had negative implications on slope stability. A sensitivity analysis developed from a theoretical hillslope will be used in order to isolate the main controls on the factor of safety. This research was presented at the American Geophysical Union Fall Meeting 2015. The oral presentation was within the session: Disturbance Hydrology: Assessing the Impact of Abrupt Landscape Changes on Watershed Hydrology.

We also have worked on the relationship between subsurface and surface characteristics, and surface fluxes like evapotranspiration (ET), one aspect that is significantly altered as a result of the mountain pine beetle infestation. We used ParFlow (PF), coupled with the Common Land Model (CLM), to model an idealized domain with homogeneous forest land cover and a heterogeneous subsurface representation of a Rocky Mountain watershed. Several scenarios with varying surface slopes and subsurface conditions were modeled to obtain annual ET distributions that were spatially-averaged at different resolutions. The average ET magnitude remained the same for each scenario regardless of the model resolution, while the standard deviation decreased with decreasing resolution. The relationship between hydraulic conductivity and ET was also found to vary with subsurface heterogeneity, anisotropy and conductivity magnitude; understanding these details, as well as the respective equations within PF-CLM that influence these relationships, is the focus of current research efforts.

Professor John McCray and PhD Student Nicolas Rodriguez worked on compiling and developing a spatially and temporally robust database to analyze the impacts of forest insect infestations on the carbon cycle in streams, and eventually other important components of the biogeochemical cycle (i.e., N, P, O). The first step after the datasets compilation to the database was to conduct rigorous geospatial and temporal statistical studies to better understand the primary variables that are most important to include in a watershed-scale hydro-chemical model wherein carbon cycling is a primary component.

The different variables included in the dataset are areas affected by Mountain Pine Beetle infestations, Spruce Beetle infestations, and other diseases; elevation; slope; aspect; fires; land cover; precipitation; temperature; snow cover; waste water treatment plant locations; wind; and soil types. The analyzed domain consisted of the mountainous region of the state of Colorado, an

Appendix F: School of Mines, Water Quality and Supply Impacts from Climate-Induced Insect Tree Mortality

area for which the USGS has more than 11000 samples of dissolved organic carbon in streams since 1970 and where bark beetle infestations have impacted the evergreen forests considerably. The temporal resolution is yearly and most of the data is being estimated back in time, as early as possible.

Ongoing research is focusing on the compilation and merging of land cover datasets. The assessment, monitoring, and characterization of land cover (LC) is essential for global change research as it is a critical variable driving many environmental processes. These tasks have become primary applications of remote sensing, resulting in increased availability of LC products. McCray and Rodriguez integrated the lines of research on space-time interpolation of a single LC product and on fusing multiple existing LC products, to produce a methodology for fusing multiple existing LC products over space and time to produce a single LC record over a long time period and a large spatial domain. Although they provide a specific illustration using six LC products over the Rocky Mountain region of the United States, the methodology can be applied to different sets of LC products to obtain a temporal set of maps with the frequency, spatial resolution, and categories required by the user.

(d) Education and outreach activities

In addition to publications in peer-reviewed journals and presentations at conferences, a panel entitled, "Hydrology and Water Quality Effects from the Mountain Pine Beetle Infestation in the Rocky Mountain West" was conducted. This panel was attended by stakeholders, water providers and consultants in the Rocky Mountain West.

The panel was held at the American Water Resources Association Annual Water Resources Conference in Denver, CO on November 16-19, 2015. These meetings target water resources professionals (providers, regulators, consultants and scientists) over the entire Rocky Mountain region. This outreach occurred in two segments: First, a traditional presentation format where five presentations from this NSF pine beetle WSC project were delivered by project PIs. The second component was a panel style discussion allowing the approximately 15 attendees to present questions to the panel. The goals of this activity were to determine previous knowledge of participants and to further public communication and general education regarding the mountain pine beetle impacts on water quality and hydrology. The activity was very successful; in addition to better education of participants on beetle impacts, priority areas of interest included: water quality, water quantity, streamflow, and increased fire risk.

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

- Bearup LA, N Bogenschuetz, CM Bokman, MM Forrester, LK Gallagher, MS Morse, JO Sharp and RM Maxwell--Math and science events at three local elementary schools (9/17/15 Mitchell Elementary; 11/4/15 Shelton Elementary; 11/12/15 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.
- MS Morse participated in classroom-based lessons at Bear Creek Elementary and at the Northglenn Water Festival. In these events, students are educated about hydrology, the water cycle and the impact of contaminants or events on the water cycle in the Rocky Mountain West using both visual and hands-on activities.

Appendix F: School of Mines, Water Quality and Supply Impacts from Climate-Induced Insect Tree Mortality

- MS Morse worked with teachers from Jefferson County, CO Public Schools Outdoor Lab at Windy Peak (Bailey, CO) to build groundwater sand tank models for use in their Outdoor Education Laboratory Program. Teachers were trained how to use the tanks to demonstrate groundwater processes to students visiting the lab. These concepts were applied to outdoor field trips with students to contextualize content from the sand tanks in a mountain setting.
- JO Sharp judged an Elementary Science Fair – January 2015 at Mitchell Elementary

Publications:

- Bearup, LA, RM Maxwell, DW Clow, JE McCray. (2014a). Hydrological effects of forest transpiration loss in bark beetle-impacted watersheds. *Nature Climate Change*. 4:481–486 (2014). doi: 10.1038/nclimate2198
- Bearup LA, Mikkelsen KM, Wiley JF, Navarre-Sitchler AK, Maxwell RM, Sharp JO, McCray JE (2014b) Metal partitioning and mobilization mechanisms in soils under bark beetle-killed trees. In review. *Science of the Total Environment*.
- Engdahl, NB and RM Maxwell (2014) Approximating groundwater age distributions using simple streamtube models and multiple tracers. *Advances in Water Resources*, ADWR2158, DOI: 10.1016/j.advwatres.2014.02.001
- Engdahl, NB (2014), Equivalence of the Time and Laplace Domain Solutions for the Steady-State Concentration of Radiometric Tracers and the Groundwater Age Equation, *Water Resources Research*, 50, doi: 10.1002/2014WR015413.
- Mikkelsen, KM, LA Bearup, AK Navarre-Sitchler, JE McCray, JO Sharp. (2014) Changes in metal mobility associated with bark beetle-induced tree mortality. *Environmental Science: Processes & Impacts* 16 (6):1318-1327. doi: 10.1039/C3EM00632H
- Mikkelsen KM, Bearup LA, Maxwell RM, Stednick JD, McCray JE, and Sharp JO (2013) Bark beetle infestation impacts on nutrient cycling, water quality and interdependent hydrological effects. *Biogeochemistry*. 115,1-21.
- Mikkelsen KM, Dickerson E, McCray JE, Maxwell RM, Sharp JO (2013) Water-quality impacts from climate-induced forest die-off. *Nature Climate Change* 3, 218-222.
- Mikkelsen KM, Maxwell RM, Ferguson I, McCray JE, and Sharp JO (2013) Mountain pine beetle infestation impacts: Modeling water and energy budgets at the hill-slope scale. *Ecohydrology* 6, 64-72.

Presentations:

- Bearup, LA and RM Maxwell. Using particle tracking to link changing streamflow

Appendix F: School of Mines, Water Quality and Supply Impacts from Climate-Induced Insect Tree Mortality

contributions to transpiration loss in bark beetle infested watersheds. International Conference on Computational Methods in Water Resources; Stuttgart, Germany, 10-13 June 2014.

- Bearup, LA and RM Maxwell. Changing stream water sources in insect-infested forests: a combined field and modeling analysis. European Geosciences Union General Assembly; Vienna, Austria, 27 April - 2 May 2014.
- Bearup LA, RM Maxwell, C Penn, DW Clow, JE McCray. Connecting increased groundwater contributions to transpiration losses in bark beetle infested watersheds. AGU Fall Meeting, San Francisco, Calif., 9-13 December 2013.
- Bearup LA, KM Mikkelsen, AK Navarre-Sitchler, RM Maxwell, JE McCray, JO Sharp. Metal Mobility in Bark Beetle-Infested Forests. GSA Annual Meeting, Denver, Colorado, 2013 Oct 27-30.
- Bearup LA, C Penn, RM Maxwell, DW Clow, JE McCray, JO Sharp. Unraveling the interconnection between hydrology and geochemistry in mountain pine beetle infested watersheds using stable isotopes and modeling. Poster at MODFLOW and More, Golden, Colorado, 2-5 June 2013.
- Bearup LA, RM Maxwell, DW Clow, JE McCray, JO Sharp. Interpreting watershed scale hydrological alterations from widespread mountain pine beetle infestation using stable isotopes. Poster at Hydrology Days, Fort Collins, Colorado, 25-27 March 2013.
- Bogenschütz N, LA Bearup, RM Maxwell, P Santi. Slope Stability Analysis of Mountain Pine Beetle Impacted Areas. Oral Presentation at AGU Fall Meeting, San Francisco, California, 14-18 December 2015.
- Brouillard B, KM Mikkelsen, E Dickenson, and J Sharp. Effects of Extensive Beetle-Induced Forest Mortality on Aromatic Organic Carbon Loading and Disinfection Byproduct Formation Potential, Poster Presentation at AGU Fall Meeting, San Francisco, California, 14-18 December 2015.
- Brouillard B, E Dickenson, and J Sharp. Seasonal Variations in Water Quality from Mountain Pine Beetle Induced Forest Die-Off. 2014 annual AWRA symposium in Golden, CO.
- Engdahl, NB, Maxwell, R.M., and Lopez, S.R. (2014) Urbanization effects on groundwater residence time distributions, 20th conference on Computational Methods in Water Resources (CMWR), June 10-14, 2014, University of Stuttgart, Stuttgart, Germany.
- Engdahl NB, and Maxwell, R.M. (2013) Realistic modeling of environmental tracer migration and composite age distributions in a pine beetle impacted watershed, Poster presentation H53F-1490, American Geophysical Union, Fall Meeting, December 9-13, 2013, San Francisco, CA.
- Engdahl, NB, and Maxwell, RM (2013), Multi-scale modeling of the effects of landscape and climate changes on integrated hydrologic systems, Oral Presentation at AGU Fall Meeting, San Francisco, California, 14-18 December 2015.
- Forrester, MM, RM Maxwell, LA Bearup, D Gochis, A Porter. Exploring the Interactions among Beetle-induced Changes in Catchment-scale Ecohydrology, Land Surface Fluxes and the Lower Atmosphere with a Coupled Hydrology-Atmospheric Model. Oral presentation T43-309-3,

Appendix F: School of Mines, Water Quality and Supply Impacts from Climate-Induced Insect Tree Mortality

Geological Society of America, Annual Meeting, October 27-30, 2013, Denver, CO

- Jefferson JL, RM Maxwell. Understanding impacts of subsurface and surface heterogeneity on evapotranspiration in mountain pine beetle infested watersheds. Poster at AGU Fall Meeting, San Francisco, Calif., 9-13 December 2013.
- Jefferson JL, RM Maxwell. Understanding impacts of subsurface and surface heterogeneity on evapotranspiration in mountain pine beetle infested watersheds. GSA Annual Meeting, Denver, Colorado, 2013 Oct 27-30.
- Mikkelson KM, LA Bearup, AK Navarre-Sitchler, JE McCray and JO Sharp. Changes to subsurface metal mobility in a bark beetle-impacted forest. 2014 annual NGWA conference in Denver, CO.
- Mikkelson KM, Will the bark beetle infestation affect water quality at water treatment plants in the Rocky Mountain West?, June 11th, 2013 AWWA conference in Denver, CO.
- Mikkelson KM, Will the bark beetle infestation affect water quality in the Rocky Mountain West?, May 14th, 2013 at the RMSWAWWA/RMWEA student conference at CSM, Golden, CO
- Mikkelson KM, Will the bark beetle epidemic impact water quality? Results from Colorado municipal water treatment facilities, February 18th, 2013 at the Institute of Arctic and Alpine Research, Boulder, CO.
- Navarre-Sitchler A, Pryhoda M, Dickenson E, Bearup L, Mikkelson K, Maxwell R, Sharp J, McCray JE. Changing soil chemistry in Rocky Mountain forests impacted by the mountain pine beetle. Goldschmidt 2014. Sacramento, CA. June 8-13, 2014
- Penn CA, RM Maxwell, NP Engdahl, DW Clow. Effects of bark beetle infestation on hydrology and land-energy feedbacks in mountain headwaters. American Geophysical Union Fall Meeting, San Francisco, CA, 9-13 December 2013
- Pryhoda MK, AK Navarre-Sitchler, E Dickenson. Pine needle leachate chemistry from trees in three stages of mountain pine beetle attack. MODFLOW and More, Golden, Colorado, 2-5 June 2013.
- Pryhoda MK, AK Navarre-Sitchler, E Dickenson. Pine needle leachate chemistry from a mountain pine beetle infested watershed in Summit County, CO. GSA, Denver, Colorado, 27-30 October 2013.
- Pryhoda MK, AK Navarre-Sitchler, E Dickenson. Impact of pine needle leachate chemistry from a mountain pine beetle infested watershed on groundwater geochemistry. AGU, San Francisco, California, 9-13 December 2013.
- Rodriguez NJ, A Hering, JE McCray. Fusing existing land cover products to produce an improved spatio-temporal record. Poster Presentation at AGU, San Francisco, California, 14-18 December 2015.
- Sharp JO, Mikkelson KM, McCray J, Maxwell R, Dickenson E. The Apple Doesn't Fall Far from the Tree: Applying Estuarine Principles to Watershed Biogeochemistry. Ocean Sciences Meeting.

Appendix F: School of Mines, Water Quality and Supply Impacts from Climate-Induced Insect Tree Mortality

Honolulu, Hawaii. Feb 23-28, 2014.

Attachment G

Engineering Research Center Reinvention of the Nation's Urban Water Infrastructure (ReNUWIt)

Colorado School of Mines

CHECRA Grant: \$400,000 (per year for 5 years, renewed)

Reporting Period: January 1 - December 31, 2015

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 climate change, population expansion, ecosystem demands and deteriorating infrastructure that threatens economic development, social welfare, and environmental sustainability. Without relatively large investments this crisis will only deepen through the 21st century. Accordingly, the goal of this ERC is to advance new strategies for water/wastewater treatment and distribution that will eliminate the need for imported water, recover resources from wastewater, and generate rather than consume energy in the operation of urban water infrastructure while simultaneously enhancing urban aquatic ecosystems. While many existing approaches could be used to transition urban water infrastructure to this more sustainable state, their implementation currently is limited by uncertainties about their long-term performance, life cycle costs, institutional impediments and public concerns about unfamiliar technologies.

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 described above, ReNUWIt has launched key research projects within three research thrust areas. These research thrust are defined as follows:

- (1) **Efficient Engineered Water Systems:** Decrease reliance on inefficient centralized treatment systems by employing distributed treatment systems that embrace water conservation, local use of alternative supplies, energy management, nutrient recovery, and that integrate with existing infrastructure;
- (2) **Natural Water Infrastructure Systems:** Integrate managed natural systems into water infrastructure to fully realize the potential benefits that natural systems can provide with respect to water storage and improvement of water quality, while simultaneously rehabilitating urban hydrology and aquatic habitat;
- (3) **Urban Systems Integration and Institutions:** Support the reinvention and restoration of urban water systems through the development of decision-making tools that account for economic, environmental and social factors and development of approaches that can circumvent impediments to change posed by regulations, laws, jurisdictional fragmentation, financing and public perception.

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 in the public, private, or academic sectors, 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 and research on engineered systems that support the concept of tailored water for distributed non-potable and potable water reuse, energy-positive wastewater treatment and nutrient recovery, concentrate management, and enhanced water recovery is being conducted.

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) to identify the most efficient scale of implementing more sustainable engineered water systems; (ii) to provide new, resilient technologies leading to energy-positive wastewater treatment and recovery of nutrients; (iii) to develop technologies that provide water tailored to meet specific needs including alternative water delivery systems; and, (iv) to develop energy-efficient hybrid systems for concentrate management and enhanced water recovery.

The thrust area on the use of *Natural Water Infrastructure Systems* will bring a much-needed quantitative approach to an area that has not previously been subjected to rigorous engineering analysis. Research at CSM will employ advances in fundamental understanding of natural systems to remove impediments to integrating natural systems into water infrastructure by making the complex processes that affect water transport, quality and ecosystem function in natural systems predictable and manageable. The goals are to: (i) develop tools for manipulating natural systems to enhance water quality; (ii) integrate managed aquifer recharge into urban settings using reclaimed water leading to drinking water augmentation; and (iii) harvest stormwater and infiltrate in urban settings to augment local supplies.

Within the *Urban Systems Integration and Institutions* thrust, research focuses on the development of integrated regional water models. These models will serve as decision-support tools for water resource and urban planners and managers to test the performance of treatment and supply options developed in the Natural and Engineered Systems thrusts.

Within the ReNUWIt framework described above, fifteen projects were funded in 2015:

- Tools to support decision making for nested, spatially-scaled, integrated urban water infrastructure (U1.2);
- Regional Demand Forecasting (U2.4);
- Denver Stormwater Planning (U2.5);
- Tailored water for distributed non-potable reuse using sequencing batch/membrane bioreactor hybrid systems (E1.1);
- Point-of-entry water treatment for potable reuse (E1.3);
- Sustainable landscape irrigation with reclaimed water (E1.5);
- Microalgae for wastewater treatment and recovery: A new approach to onsite wastewater treatment (E2.2);
- Anaerobic digestion as primary treatment at WWTPs (E2.4);
- Hydrothermal Technologies: Energy-positive wastewater treatment and resource recovery (E2.12, new project in 2015)
- Design of unit process wetlands to optimize chemical contaminant removal (N1.2);
- Managed aquifer recharge and recovery: Simulation, modeling and operation (N2.1);
- Improving water quality during managed aquifer recharge (MAR) (N2.2)

- Aquifer storage, treatment, and harvesting of stormwater for distributed reuse: coupled modeling, laboratory and field studies (N3.1);
- Methodologies, models, and materials for predictable removal of chemicals from stormwater during distributed recharge (N3.3); and
- Hyporheic zone management for water quality improvement (N3.4).

Principal Investigators	Funding from CHECRA
John McCray, CSM Principal Investigator Center Lead Project co-Lead, Denver Stormwater Planning, U2.5	\$12,828 \$17,580
Tzahi Cath Project Lead, Tailored Water, E1.1 Project Lead, Microalgae Wastewater Treatment, E2.2	\$35,428 \$20,235
Linda Figueroa Project Lead, Anaerobic Digestion, E2.4	\$14,789
Christopher Higgins Project Lead, Subsurface Purification, N3.3	\$18,441
Terri Hogue Project co-Lead, Denver Stormwater Planning, U2.5	\$17,580
Reed Maxwell Project Lead, Coupled Modeling, N3.1	\$49,886
Jonathan Sharp Project Lead, Unit Process Wetland, N1.2 Project Lead, Unit Process Recharge, N2.2	\$6,532 \$42,809
Kathleen Smits Project Lead, Aquifer Management, N2.1	\$985
TOTAL SPENDING (Jan-Dec 2015)	\$273,093

Within the ReNUWIt projects (2015), full or partial support was provided to:

- 11 Doctoral students
- 6 Master's of Science Thesis students
- 2 Hourly Graduate Students, Non-thesis Master's Students
- 14 Hourly Undergraduate students
- 4 REUs ~ a 10 week summer program designed to provide research experience for undergraduates
- 1 Post Doctoral Fellows
- 3 Assistant Research Faculty
- 2 Research Staff
- 13 Faculty ~ 3 Assistant Professors; 5 Associate Professors; and 5 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; design and installation of new testing apparatus; 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 tuition and nominal materials for a MS student while the student stipend/salary was contributed in-kind by Denver Water (U2.5).

Tzahi Cath, Associate Professor: Funding for one graduate student focused on energy optimization and tailored non-potable reuse (E1.1). Partial funding for one graduate student focused on gasification for energy recovery from wastewater solids (E2.2).

Linda Figueroa, Associate Professor: Tuition support for a graduate student who is developing a pilot-scale reactor for methane recovery 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 analysis of samples from the pilot scale anaerobic bioreactor at Plum Creek Wastewater Authority. In-kind support was provided by Plum Creek Wastewater Authority for student salary and analysis.

Christopher Higgins, Associate Professor: One graduate student is developing special adsorbants to remove chemical contaminants in stormwater during distributed recharge (N3.3). Support for the graduate is through a NSF Scholarship. CHECRA funds supported one hourly undergraduate student and partially supported one post doctoral fellow to assisting chemical analysis using liquid chromatography tandem mass spectrometry (LC-MS/MS). Partial faculty salary support was provided for student advising and mentoring.

Terri Hogue, Professor: One undergraduate student was supported for hydrologic modeling of the Berkeley neighborhood in northwest Denver and one undergraduate student was supported for data gathering and synthesis required by the model.

Reed Maxwell, Professor: One graduate student was also supported looking at water quantity impacts of converting pervious areas to low impact development in urbanized watersheds (N3.1). Specifically looking at 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. Partial faculty salary support was provided for student advising and mentoring.

Jonathan Sharp, Associate Professor: Partial salary support was provided to one research assistant professor to evaluate attenuation of trace organic chemicals in managed aquifer recharge systems (N2.2). Partial salary support was for student advising and mentoring.

Kathleen Smits, Assistant Professor: Nominal support for materials to complete the project on managed aquifer recharge (N2.1).

Results Achieved

Center scientists and engineers continued field research at Colorado School of Mines campus test bed that utilizes and treats municipal wastewater (~7,000 gal/day) to support both the *Efficient Engineered Water Systems* and *Natural Water Infrastructure Systems* thrusts. 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.

Specific to *Efficient Engineered Water Systems*, 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, application of reclaimed wastewater to fertigation (which decreases the amount of nutrient removal required) can benefit wastewater utilities. A third season of irrigation, analyses of leachate, and soil samples collection was completed to assess using tailored water for irrigation to reduce potable use, reduction of mineral fertilizers, and minimize nitrate leaching to groundwater.

We have developed a methodology that uses multivariate statistical process control (MSPC) to improve systems operation of wastewater treatment systems by identifying needed changes in design variables. This system will result in energy, time, and money savings in addition to improved treatment performance (e.g., higher water quality output). These results lead to award of a new \$1.2M grant through KAUST titled "Statistical Process Monitoring and Risk Assessment for Engineering and Spatial Environmental Applications."

Demonstration scale anaerobic baffled reactors have been operating at the Plume Creek Water Reclamation Authority (PCWRA) in Castle Rock for three 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.

Activities within the *Natural Water Infrastructure Systems* thrust included the upscaling of testing at the field scale. CSM investigators helped to design an open water wetlands cell constructed at Prado by the Orange County Water Department, and installed a new testbed to install water treatment features in streambeds for treating storm-water pollutants and promote cleaner water leaving our cities. These modules were termed "Biohydrochemical Stream Water Treatment (BEST)" modules and an invention disclosure has been filed at CSM.

Researchers are working to develop smarter, more efficient methods for infiltrating recycled water for aquifer storage while simultaneously improving water quality. Our work on managed aquifer recharge and engineered wetlands is of benefit to the growing urban and periurban communities in the Colorado Front Range as it directly addresses important issues such as water imports (e.g., from beyond the continental divide) as well as energy demand for import, storage and treatment. These sustainable technologies capitalize on the management of natural treatment processes to facilitate water treatment while enhancing storage infrastructure. Elements of this work also transcend the important topic of drinking water sustainability and treatment and are relevant more broadly to surface and subsurface water quality and natural treatment of impaired waters such as might be influenced by industry and resource extraction processes (i.e. oil and minerals) so important to the economy and long term well being of Colorado residents.

New geomedia is also being researched for the potential to remove stormwater pollutants during infiltration in engineered low-impact development (LID features). We are working on a plan to do a small in-field BioCHARGE test bed at the Denver Botanic Gardens. In addition, 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.

Within the *Urban Systems Integration and Institutions* thrust, CSM center scientists and students are working in collaborations focusing on stormwater planning, management and treatment. In partnership with the City and County of Denver a 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.

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 has been 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 2015. These funds in combination with CHECRA funds and \$119,472 CSM matching funds have supported:
 - 18 graduate students (tuition and stipend) in the first 4 years of ReNUWIt (2011-2015) with degrees in Civil & Environmental Engineering, Hydrologic Science and Engineering, Geological Engineering, and Applied Math and Statistics. Women comprised 55% of these graduate students, and several were ethnic minorities. Most of these students will enter the Colorado STEM workforce.
 - Research experiences for 19 Mines undergraduates in 5 different degree programs at Mines. 58% of these students were female, and several were underrepresented ethnic minorities. 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. Current relationships exist with Shelton Elementary, Ralston Elementary, Free Horizon Montessori, Wheat Ridge 5-8, Englewood Middle School, and Englewood High School. Partnerships for planned activities include Mitchell Elementary, Pleasant View Elementary, Welchester Elementary, Kyffin Elementary, Bell Middle School, Golden High School, and Jefferson 7-12.
 - Our CHECRA-funded educational efforts have led to additional funds to create an REU site (summer research for undergraduates) for ReNUWIt on the 4 campuses, and also an NSF Research Experiences for Teachers (RET) site (summer STEM education and teaching methods for K-12 and community college teachers) on the Mines campus.

- 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.
- In collaboration with the City and County of Denver, the Urban Drainage and Flood Control District (UDFCD), and Enginuity Engineering Solutions, we are evaluating how low impervious design (LID) impacts on urban flooding using high resolution models. The goal is to make recommendations on how the City can incorporate LIDs as a viable alternative in master planning for improved water quantity and quality.
- 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.
- 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 2015 (funded wholly or in part with CHECRA funds):

Thesis and Dissertations:

Carandang, C. (2015). Evaluating Impacts of Drought and Conservation Measures on Urban Vegetation in Southern California. M.S. Thesis. Civil and Environmental Engineering, Colorado School of Mines, Golden, CO.

Drumheller, Z. (2015). Development of a Simulation-based Control Optimization Algorithm with Dynamic Uncertain Parameter Inversion for Stochastic, Nonlinear Systems Containing Time Delay: A Proof-of-Concept Applied to Managed Aquifer Recharge and Recovery. M.S. Thesis. Civil and Environmental Engineering, Colorado School of Mines, Golden, CO.

Holloway, R. (2015). A Comprehensive Assessment of a Hybrid Ultrafiltration-Osmotic Membrane Bioreactor for Potable Reuse and Nutrient Removal from Municipal Wastewater. Ph.D. Dissertation. Civil and Environmental Engineering, Colorado School of Mines, Golden, CO.

Leveraged with CHECRA but no direct funds:

Coday, B. (2015). Engineered Osmosis Technology for Desalination of Oil and Gas Exploration Wastewaters: Assessment of Membrane Performance and Process Sustainability. Ph.D. Dissertation. Civil and Environmental Engineering, Colorado School of Mines, Golden, CO.

Radavich, K. (2015). Assessing the Effect of Best Management Practices on Water Quality and Flow Regime in an Urban Watershed under Climate Change Disturbance. M.S. Thesis. Civil and Environmental Engineering, Colorado School of Mines, Golden, CO.

Publications:

- Blaine, A. C., Rich, C. D., Sedlacko, E. M., Hyland, K. C., Stushnoff, C., Dickenson, E. R. V., & Higgins, C. P. (2014). Perfluoroalkyl acid uptake in lettuce (*Lactuca sativa*) and strawberry (*Fragaria ananassa*) irrigated with reclaimed water. *Environmental science & technology*, 48(24), 14361-14368. doi:10.1021/es504150h
- Chaudhry, R. M., Nelson, K. L., & Drewes, J. r. E. (2015). Mechanisms of pathogenic virus removal in a full-scale membrane bioreactor. *Environmental science & technology*, 49(5), 2815-2822. doi:10.1021/es505332n
- Chaudhry, R. M., Holloway, R. W., Cath, T. Y., & Nelson, K. L. (2015). Impact of virus surface characteristics on removal mechanisms within membrane bioreactors. *Water Research*, 84, 144-152. doi:10.1016/j.watres.2015.07.020
- DiPalma, M., Rauch-Williams, T., Fraser, J., & Munakata Marr, J. (2014). Operational Strategies for Promoting Nitrogen Elimination in Centrate Side Stream Treatment. Proceedings of the Water Environment Federation, 2014(9), 5206-5214.
- Hahn, M. J., & Figueroa, L. A. (2015). Pilot scale application of anaerobic baffled reactor for biologically enhanced primary treatment of raw municipal wastewater. *Water Research*. doi:10.1016/j.watres.2015.09.027
- Herzog, S., Higgins, C. P., & McCray, J. E. (2014, May 5). Streambed Hydraulic Conductivity Structures: Enhanced Hyporheic Exchange in Model and Constructed Stream. *Paper presented at the NGWA Groundwater SUMMIT*.
- Herzog, S. P., Higgins, C. P., & McCray, J. E. (2015). Engineered Streambeds for Induced Hyporheic Flow: Enhanced Removal of Nutrients, Pathogens, and Metals from Urban Streams. *Journal of Environmental Engineering*, 04015053. doi:10.1061/(ASCE)EE.1943-7870.0001012
- Hogue, T. S., & Pincetl, S. (2015). Are you watering your lawn? *Science*, 348(6241), 1319-1320. doi:10.1126/science.aaa6909
- Holloway, R. W., Achilli, A., & Cath, T. Y. (2015). The osmotic membrane bioreactor: a critical review. *Environmental Science: Water Research & Technology*, 1(5), 581-605. doi:10.1039/C5EW00103J
- Holloway, R. W., Maltos, R., Vanneste, J., & Cath, T. Y. (2015). Mixed draw Solutions for Improved forward osmosis performance. *Journal of Membrane Science*. doi:10.1016/j.memsci.2015.05.016
- Holloway, R. W., Wait, A. S., da Silva, A. F., Herron, J., Schutter, M. D., Lampi, K., & Cath, T. Y. (2015). Long-term pilot scale investigation of novel hybrid ultrafiltration-osmotic membrane bioreactors. *Desalination*, 363, 64-74. doi:10.1016/j.desal.2014.05.040
- Hyland, K. C., Blaine, A. C., Dickenson, E. R. V., & Higgins, C. P. (2015). Accumulation of contaminants of emerging concern in food crops, part one: Edible strawberries and lettuce grown in reclaimed water. *Environmental Toxicology and Chemistry*. doi:10.1002/etc.3066
- Hyland, K. C., Blaine, A. C., & Higgins, C. P. (2015). Accumulation of contaminants of emerging concern in food crops, part two: Plant distribution. *Environmental Toxicology and Chemistry*. doi:10.1002/etc.3068
- Kinoshita, A. M., & Hogue, T. S. (2015). Increased dry season water yield in burned watersheds in Southern California. *Environmental Research Letters*, 10(1), 014003. doi:10.1088/1748-9326/10/1/014003
- Kirsch, B. R., & Maxwell, R. M. (2015). The Use of a Water Market to Minimize Drought-Induced Losses in the Bay Area of California. *Journal - American Water Works Association*, 107(5), E274-E281.
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Appendix H.1

MRI: Acquisition of a Single Crystal X-Ray Diffractometer

University of Northern Colorado

NSF Grant CHE-1428630

PIs Robert P. Houser, Robin Macaluso, and Michael Mosher

Total 2015 CHECRA funding \$93,783

Project description and principal personnel involved:

Overview – Funds were requested to purchase a Bruker D8 Quest single-crystal X-ray diffractometer (XRD) to support ongoing faculty research and development, undergraduate and graduate research and research training in the Departments of Chemistry and Biochemistry at the University of Northern Colorado (UNC), the University of Nebraska at Kearney, and the Colorado School of Mines.

The goal of this project is to enhance emerging faculty research and allow us to engage undergraduate, graduate and postdoctoral researchers in exciting, cutting-edge research involving techniques not previously available at UNC. The XRD will advance the research efforts of multiple research laboratories at UNC, in Northern Colorado, and in the region. The acquisition of a single-crystal XRD at UNC will enhance the productivity of research groups who are pursuing wide-ranging areas of chemistry, biochemistry, and materials science. These research activities span diverse topics ranging from novel magnetic frustration in intermetallic compounds to isoxazole heterocycle-DNA interactions.

Instrument purchase and installation: The XRD was purchased from Bruker and installed in January 2015. The instrument is housed in a dedicated room in Ross Hall on the UNC campus, and appropriate supervision and training will be provided to encourage wide use of the XRD in research and training.

Scientific impact: Structural characterization of new molecules and materials synthesized at UNC and surrounding institutions will provide critical data that will help to solve problems in areas ranging from solid-state materials, organic, inorganic, and biological chemistry. Previously, the resources for single-crystal X-ray analysis were inadequate in Northern Colorado.

Research in PI Houser's laboratory focuses on transition metal coordination chemistry related to questions in bioinorganic and coordination polymers chemistry. Houser will investigate the redox chemistry of thioether amide ligands with copper(II) to gain insight into the oxidation of methionine in biological electron transfer and neurological diseases such as Parkinson's and Alzheimer's diseases.

PI Macaluso left UNC for a faculty position at the University of Texas, Arlington.

PI Mosher studies structural characteristics of substituted acridines and their interactions within biological systems. Binding studies of 9-anilinoacridines with double-stranded DNA indicate that specific geometries are necessary for enhanced association of these drugs with the DNA. The resulting intercalator-linker-minor groove binders were found to exhibit antitumor activity in screens performed by the National Cancer Institute and has since led to the development of more active compounds for the treatment of cancer.

Eric Toberer (Colorado School of Mines, major user) is actively pursuing single crystal growth and characterization of photovoltaic and thermoelectric materials. In both cases, the Toberer group is interested in developing non-traditional semiconductors for these applications. For nontraditional photovoltaics, such as top-cell materials for Si-based tandems, it is critical to understand the *intrinsic* material properties of quality *single crystals* to serve as a baseline for understanding thin films.

Haishi Cao (University Nebraska-Kearney, major user) is interested in developing specific sensors for fluorescence detection of bio-related molecules to investigate their roles in the biological processes. Current interests focus on sensors for fructose-6-phosphate (F6P), which stems from the role of F6P in carbohydrate metabolism. □ The single crystal XRD will be the major means of investigation the binding properties between sensor and F6P to explain the binding affinity and molecular selectivity.

Educational impact and outreach: Because UNC is a comprehensive institution of higher education, integrating modern instrumentation into research and learning opportunities is highly valued. The single-crystal X-ray diffractometer will be central to the development of several courses that address a variety of students to maximize the impact of the instrument.

The XRD will provide research and educational experiences for undergraduates, graduate students, postdoctoral fellows, and high school teachers and students, many of whom will be □trained to gain hands-on experience with crystallography. Undergraduate, graduate, postdoctoral researchers and faculty will benefit from hands-on experience with the single-crystal XRD. The instrument will □be integrated into a variety of undergraduate laboratory and graduate-level courses. Through these activities, college undergraduates, graduate students, and postdoctoral researchers will be trained in □the use of state-of-the art crystallographic methods in the characterization of their compounds. Furthermore, through the outreach and training of high school teachers, modern scientific methods and concepts will be used in teaching their students, thus enhancing their students' education in chemistry and physics.

Appendix H.2

MRI: Acquisition of a High Performance Computing Cluster for Multidisciplinary Research and Education

University of Northern Colorado

NSF Grant ACI-1429003

PIs Mehrgan Mostowfi, Seth Fietze, Wendilyn Flynn, David Hydock, and David Lerach

Total 2015 CHECRA funding \$ 59,978

Project description and principal personnel involved:

Overview – Funds were requested to acquire a broadly accessible High Performance Computing (HPC) cluster to support the research and education programs at the University of Northern Colorado (UNC). The instrument will be utilized by researchers from a number of disciplines, including biology, computer science, exercise science, mathematics and earth and atmospheric sciences. This instrument will allow faculty to expand and strengthen ongoing collaborative research programs and to incorporate faculty research into research training courses for undergraduates and graduate students. The project PIs and collaborators have experience in the use of computation clusters and incorporation of students into research-based training opportunities. The management and sustainability plans provide for effective and equitable sharing of the instrument, as well as upgrades and continued operation into the future.

The goal of this project is to enable scientific progress across a spectrum of investigations ongoing at UNC that was previously hampered by the lack of large-scale modern computational resources. The establishment of a centralized computational and storage resource for a diverse set of campus users will provide a rich and useful resource for collaboration, not just for individual research projects, but also for the existing intellectual environment at UNC (and its collaborators). The computing cluster will significantly strengthen interdisciplinary graduate research in the School of Biological Sciences at UNC, and will also strongly contribute to interdisciplinary curricular development designed to increase the numbers undergraduates completing degrees in the sciences and mathematics at UNC.

Instrument purchase and installation: The HPC cluster was purchased and installed in the UNC Carter Hall datacenter in October 2015, and became operation in December of 2015. The cluster is managed by Information Management & Technology (IM&T), which is the primary information technology provider at UNC. We anticipate that during the first year of operation (2016), the number of cluster users will be limited to the PIs, major users, and researchers

directly collaborating with them on their research projects. The majority of the hardware maintenance needed for the cluster will be performed by the UNC IM&T. Non-routine maintenance will be administered by the vendor as needed.

Scientific impact: The HPC cluster will support research in bioinformatics and genomic research, computer science and earth and atmospheric research UNC. Our aim is to establish computational research resources on campus and to make these resources available to all of UNC. The HPC cluster will serve to facilitate important opportunities for cross discipline collaborations in the research and educational areas described here.

PIs Hydock (Exercise Science) and Fietze (Biological Sciences) seek to apply computational and experimental approaches to dissect the topology and regulatory principles of molecular and cellular circuits (e.g., circuits involving interactions among genes, cells, proteins, and drug treatments).

PI Mostowfi (Mathematics and Computer Science) will use the HPC cluster in order to build system prototypes of new traffic shaping methods to increase the energy efficiency of networked devices. The focus is on methods for individual devices. However, when multiple devices utilize these methods, a wide-spread effect can propagate in the network.

PIs Flynn and Lerach (Earth and Atmospheric Sciences) will set up a high-resolution daily operational weather forecast model to be run on the cluster using the Regional Atmospheric Modeling System (RAMS) version 6.0 to be used for the creation of sophisticated, high resolution weather forecasts for the state of Colorado, and specifically, along Colorado's Front Range. RAMS incorporates a two-moment bulk microphysics scheme that predicts the mixing ratio and number concentration of cloud droplets, drizzle, rain, pristine ice, snow, aggregates, graupel, and hail. In addition, cloud nucleation by both ice and cloud condensation nuclei (aerosol particles) are explicitly considered.

Educational impact and outreach: Our primary goal is to increase scientific computing literacy in our graduates by providing more students with meaningful quantitative research experiences and maximizing integration of faculty research with science education. The addition of the HPC cluster to our university will significantly increase our research productivity, enhance collaborations with colleagues at other professional institutions, and ensure modern computing experiences for hundreds of undergraduate and graduate student researchers-in-training each year. The importance of integrating current computing skills into a research-infused curriculum cannot be overstated, especially in an age when all scientific, engineering, scholarly, educational activities are deeply impacted by developments in information technologies. Additionally, the development of new courses, expanded research experiences for graduate and undergraduate students, and developing hand-on computational workshops for high school students and K-12 science teachers (through UNC's Frontiers of Science and Math and Science Teaching Institutes) are an integral part of planned use of the UNC HPC Cluster.

Attachment H.3

MRI: Acquisition of a coupled optical and scanning probe microscopy facility for advanced materials research

Colorado School of Mines

CHECRA Grant: \$60,000

Reporting Period: January 1 - December 31, 2015

Summary: Colorado School of Mines (CSM) was awarded a National Science Foundation (NSF) Major Research Instrumentation (MRI) award to acquire a coupled optical and scanning probe microscopy facility for advanced materials research. This award will create a self-sustaining scanning probe microscopy (SPM) facility with unique capabilities for advanced materials research at the CSM). This instrumentation request includes an atomic force microscope (AFM) coupled to an optical microscope for simultaneous imaging and physical properties measurements at the nanoscale for a wide range of advanced materials in renewable energy and life sciences. This facility, under the leadership of Professors Colin Wolden and Keith Neeves, is designed to serve a multi-user environment and will be operated in a shared-use facility, with participation from the majority of departments across campus as well as our regional partners the National Renewable Energy Laboratory (NREL) and Children's Hospital Colorado (CHC). We will organize and host an annual Rocky Mountain Scanning Probe Microscopy Workshop to provide training opportunities and attract new regional users to the facility beyond our partners at NREL and CHC. Undergraduates will be introduced to SPM through our existing summer REU programs.

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

The CHECRA grant was used to supply part of the required matching funds that in combination will create a scanning probe microscopy facility valued \$351,000. The NSF made the award on September 15th, 2015. In the final quarter of 2015 we designed and specified the requirements both the optical microscope and the scanning probe. After proceeding through the State of Colorado mandated procurement processes final purchase orders were released in December 2015, and we expect delivery and assembly of the facility to occur in March 2016. .

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

The CHECRA funds (\$60,000) will be used exclusively to purchase the equipment for the SPM facility.

Results Achieved

None to date.

Summary of Benefits to the State of Colorado

- Received \$245,878 in NSF core funds in 2015.

Publications and Presentations in 2015 (funded wholly or in part with CHECRA funds):

None to date

Presentations:

None to date

Appendix H.4

MRI Collaborative Consortium: Acquisition of a Shared Supercomputer by the Rocky Mountain Advanced Computing Consortium

NSF award to University of Colorado, Boulder (UCB), Award 1532236

Total 2015 CHECRA Funding - \$140,000

Award PI's – Thomas Hauser, Anna Hasenfratz, James P. Syvitski, Kenneth E. Jansen, Peter A. Ruprecht

NSF award to Colorado State University, Award 1532235 (This award is in collaboration with the UCB award)

Award PI - Howard Jay Siegel

\$2,030,000 was awarded for equipment only to CU-Boulder and \$700,000 to CSU as part of the collaborative proposal. The total amount allocated for the supercomputer is \$3,600,000 million taking the required matching of 30 percent into account.

A cluster supercomputer will be deployed by the University of Colorado Boulder (CU-Boulder) and Colorado State University (CSU) for the Rocky Mountain Advanced Computing Consortium (RMACC). This high-performance computing (HPC) system supports multiple research groups across the Rocky Mountain region in fields including astrophysics, bioinformatics, chemistry, computational fluid dynamics, earth system science, life science, material science, physics, and social sciences with advanced computing capabilities. It also provides a platform to investigate and address the impact of many-core processors on the applications that support research in these fields.

CU-Boulder and CSU have gone through a competitive bid process and issued a joint purchase order to Dell for a supercomputer. Right now the CU-Boulder team is working on the preparation of the data center and working with the vendor on a deployment plan.

Benefits to the region: The proposed system integrates nodes populated with Intel's conventional multicore Xeon processors and Many-Integrated-Core (MIC) 'Knights Landing' Phi processors interconnected by Intel's new Omni-Path networking technology. Users of the new HPC system have access to existing data management services including data storage, data sharing, metadata consulting,

and data publishing, leveraging the NSF-funded high-performance networking infrastructure and long term storage system, as well as additional cyberinfrastructure, at CU-Boulder and CSU. The many-core feature of this HPC system enhances graduate and undergraduate students' education and training as they develop, deploy, test, and run optimized applications for next generation many-core architectures. Training for researchers and students is provided through workshops appropriate for introducing diverse audiences to the efficient and effective use of HPC systems, the challenges of vectorization for single core performance, shared memory parallelism, and issues of data management. Additionally, advanced workshops on large-scale distributed computing, high-throughput computing, and data-intensive computing are offered during the year and at the annual RMACC student-centric HPC Symposium. The Symposium brings together hundreds of students, researchers, and professionals from universities, national laboratories and industry to exchange ideas and best practices in all areas of cyberinfrastructure. For-credit HPC classes will be delivered for online participation, educating the next generation of computational scientists in state-of-the-art computational techniques.

Appendix H.5

Infrared scanning near-field optical microscope (IR s-SNOM) for broadband nano-imaging and -spectroscopy

NSF Grant 1531996

PIs Markus B. Raschke, Prashant Nagpal, Sean E. Shaheen, Steven T. Cundiff, Thomas T. Perkins

Total 2015 CHECRA funding \$80,000

Project description and principal personnel involved:

Overview - Heterogeneity defines the properties of most functional molecular materials. Their specific catalytic, biological, electronic, optical, or photophysical properties arise from defined *spatial* distributions, morphologies, and structures of the different chemical constituents. The associated *coupling* and resulting functional interactions are defined on nanometer length scales determined by electron or structural correlations. Infrared vibrational nano-imaging and -spectroscopy has emerged as a potentially transformative technique at the frontier of imaging science because of its unique ability for *local probing* of the molecular or nanostructure environment with chemical sensitivity and nanometer spatial resolution. ***Nano-scale spectroscopic imaging*** thus gives access to material systems characterized by a high level of heterogeneity with multicomponent interactions, whose understanding has traditionally been limited due to a lack of suitable chemical imaging techniques to provide the desired molecular level insight.

The goal of this project is to develop an instrument for broadband and broadly tunable infrared vibrational scattering-scanning near-field optical microscopy (IR s-SNOM) for chemical nano-imaging and spectroscopy on the molecular scale. The instrument is being developed based on enabling technical innovations by Markus Raschke as principal investigator. The instrument will meet a pressing need in chemical nano-imaging materials, photonics, biological, and geochemical processes defined on molecular length scales. This approach will foster true synergies in research, development, education, and training in the emergent ***frontier of imaging science***.

The instrument will be made available as a *collaborative research facility* to assist a wide range of researchers across campus and collaborators at different institutes in Colorado as well as industry to achieve a wide range of research and development goals. The instrument will provide much needed chemical imaging with nanometer spatial resolution, high spectral resolution, small ensemble to

single molecule sensitivity, and operation under *in situ* and aqueous environments.

Instrument development and commissioning is projected over a three-year period, with first prototype performance and use expected as early as end of 2016. With a project start in October 2015, by end of the reporting period 2015 it is still in an early planning stage.

As of December 31, 2015 the following goals have been achieved: A senior research associate, Dr. Bernd Metzger, has been hired to lead the instrument development. Dr. Metzger has leading expertise in nonlinear nano-optics and laser source development. He has started to research different optical designs and performed modeling and first testing of some signal detection schemes.

Scientific impact: The expected instrument performance provides for **systematic investigations of the microscopic processes that control complex and multicomponent molecular matter on its elementary level.** The instrument development effort is driven by a wide range of application needs, including coupling and transport in organic photovoltaics and electrochemical transistors, access of structure and function of membrane proteins, to investigate intersubband transitions in nano-bio-hybrid materials for solar fuel generation, and to probe intermolecular coupling and dynamics through local probe vibrational solvatochromism.

Industrial and educational impact and outreach: The instrument will serve 10 research groups and collaborators, with combined >40 students from 6 different departments at the University of Colorado, NIST, and NREL, for studies of soft-matter heterostructures, driving forces in new liquid crystal structure themes, control of electronic structure and adsorbates on 2D nanomaterials and at interfaces, geo-microbial systems, and biomineralization.

Based on these applications it will provide a platform for collaborative and interdisciplinary research and training activities around the instrument.

In addition the IR s-SNOM instrument will have broad impact in different industries. The photonic and laser industry contributes and benefits with novel laser and pulse shaping concepts. The biomedical and diagnostics industry has expressed need in its capability for nano-scale chemical materials characterization. Moreover, students trained in the new imaging technology will be a highly trained workforce to join these technology industries.

The instrument will be integrated into the Nanoscale Characterization lab (NCL) and the Soft Materials Research Center (MRSEC) and be available for shared use. Teaching modules will be developed for different nano-science and -imaging courses, in combination with interdisciplinary research and education programs on campus, including the REU program in physics, NSF IQ-Biology-IGERT, and the NIH Molecular Biophysics Training Program. These programs already promote a culture of interdisciplinary research and training, including increased participation from minorities and women.

**Attachment H.6: Colorado State University
Acquisition of Combined Spinning Disc Confocal/Atomic Force Microscopy System**

CHECRA Report for 2015

Principle Investigator: Matt Kipper

Co-Principle Investigators: Kiego Krapf, Susan James

CHECRA Grant:

Project Description:

The objective of this project is to acquire a new microscopy system that combines multiple techniques in a single platform. This instrument will be housed in a facility that enables secure 24-hour access for users and will be maintained by a staff scientist. The instrument will be included in a new module for an undergraduate lab course that serves about 100 students annually. Students in a graduate course on microscopy will also be introduced to the instrument. The instrument will be made available to a broad user base both inside and outside of CSU, by including it in a Microscopy Imaging Network (MIN).

The instrument will combine scanning probe and optical techniques. The scanning probe techniques enable imaging of the topographical features and mechanical properties of samples at very high resolution. The optical techniques include spinning disc confocal microscopy, fluorescence recovery after photobleaching (FRAP), and photoactivation (PA). The instrument will be configured to perform imaging of wet samples including live cells. Combining these fundamentally different yet complementary techniques on a single platform enables interrogation of multiple sample properties simultaneously and in the exact same field of view. Therefore specific measurements made with one technique (e.g. mechanical properties) can be correlated with features (e.g. location of chemical functional groups or biological structures) measured by another technique. Changes in these correlations and spatial organization can be monitored over time to observe biological phenomena. The initial user group consists of 19 investigators in ten academic departments from three universities (CSU, University of Colorado at Denver, and University of Denver). These investigators will use the instrument for interdisciplinary and collaborative research projects including biochemical and biophysical studies and for the development of new materials for biomedical and tissue engineering applications.

How funding was applied:

This award contributes a major portion of the matching funds required to apply for a Major Research Instrumentation (MRI) grant from the National Science Foundation (NSF). This funding mechanism requires a 30 % cost-share from the awardee. The total project budget is \$912,853. \$638,997 was requested from the NSF; CHECRA funds were used to partially satisfy the required \$273,856 of obligatory cost sharing.

Results:

We were successful in obtaining funding from the NSF, totaling \$638,997. The final configuration of the instrument, including spinning-disc inverted optical microscope, FRAP and PA components, acoustic and vibration isolation, and scanning probe microscope components were established in fall 2015. Final purchase orders were sent to four vendors in January and February 2016 to acquire all components of the instrument. We anticipate delivery of all components by the end of March, 2016. The instrument will be installed in April 2016. The instrumentation purchased includes:

- Nikon Ti-E Perfect Focus inverted optical microscope, including motorized wide-field fluorescence components, Yokagowa CSU-X1 spinning disk, CCD camera, laser launch, galvo-based point scanner, computer, monitor, and software.
- Bruker Bioscope Resolve Scanning Probe Microscope, peak-force QNM nanomechanics package, fast force-volume software, image registration and overlay software for integrating

images from the optical microscope, microvolume sample cell, heating stage, perfusion stage incubator, and computer monitor.

- Technical Manufacturing corporation optical table.
- Herzan AEK-2011 Acoustic isolation enclosure.

Attachment H.7: Colorado State University -- Development of a Ship-based C-Band Polarimetric Radar

PI: Prof. Steven A Rutledge, CO-PI: Prof. V. Chandrasekar

CHECRA funds allotted to project: \$125,000

Project Summary

This project is concerned with building a state of the art, polarimetric C-band Doppler radar to be deployed periodically on world-class research ships to study oceanic precipitation systems. Oceanic precipitation, especially in the tropics, plays a central role in driving our planet's weather. Furthermore, to better understand the role of tropical rainfall in climate change, it is paramount to better understand the physical nature of this rainfall. The radar, known as SEA-POL, will play a crucial role in such studies. CSU received a highly competitive Major Research Instrumentation grant from the National Science Foundation to build this radar system, "Development of a Ship-based C-band Polarimetric Radar". The overall funding for this project consists of the \$917,836 NSF grant, a \$125,000 contribution from the Colorado Higher Education Competitive Research Authority (CHECRA), and a \$268,358 cost sharing contribution from Colorado State University.

Description of the project, the principal persons or entities involved

Professors Steven Rutledge and V. Chandrasekar are leading the project along with assistance from Engineers Francesc Junyent and Jim George, Radar Technician Bob Bowie and Graduate Research Assistant Alex Morin. Several years ago NOAA donated the R/V Ronald C. Brown C-band radar to the Department of Atmospheric Science at CSU. Our project utilizes several key components from this radar; the C-band magnetron transmitter and the antenna pedestal and radome. The project will acquire a new antenna, and a state of the art signal processor and receiver system, along with several other key electrical components. The radar electronics will be housed in two new seaintainers, facilitating installation on ships and easy transport to various ports around the world.

Amount of funding allocated to each principal person or entity, manner in which each entity applied the funding in connection with the project and results achieved

The \$125,000 in state matching funds for "Development of SEA-POL, a Ship-based C-Band Polarimetric Radar" will be used primarily to support the fabrication costs associated with the radar. This includes salary for the Graduate Research Assistant, Engineers and Technician, as well as fabrication materials for the radar.

Personnel:		CHECRA Funds
<i>Junyent, Francesc</i>	<i>Engineer</i>	\$ 3,491.00
<i>George, Jim</i>	<i>Engineer</i>	\$ 3,491.00
<i>Bowie, Bob</i>	<i>Technician</i>	\$ 7,758.00
<i>Morin, Alex</i>	<i>GRA</i>	\$ 2,133.00

<i>Fringe</i>	\$ 3,935.00
Fabrication Materials	<u>\$ 104,192.00</u>
Total CHECRA funds	<u><u>\$ 125,000.00</u></u>

Results achieved by the project (summary of benefits to the State of Colorado)

We have finished detailed CAD designs of the overall radar and all sub-assemblies. We are now working with CSU Purchasing to establish vendor contracts for the signal processor/radar receiver system, and the seatainers. Purchase of the new antenna system will follow soon. We have established a detailed timeline for the radar assembly and testing period. We anticipate having the radar configured for detailed testing by February 2017.

It is expected that the radar will be utilized in several high profile tropical field projects beginning in late summer 2017 and running through late 2018. A proposal for one of these projects (totaling \$2.9M over a four year period) has already been submitted to the Office of Naval Research. These monies would come directly to CSU to create positions for new staff and graduate students.

When SEA-POL is not deployed at sea, it will operate at the CSU-CHILL National Radar Facility site in Greeley CO. As such, SEA-POL will support studies of severe storms to help improve warning procedures for severe weather, such as those routinely provided to the public. SEA-POL will also be an integral component of graduate classes in atmospheric science and electrical engineering, therefore enhancing classroom learning for our students.

The SEA-POL project is on schedule and with no significant problems at this time.