

Attachment A

Renewable Energy Materials Research Science and Engineering Center

Colorado School of Mines

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

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 are nearly ten times 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 is concentrating on materials of potential use in the next generation of PV devices, but the scope of this IRG will be 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 is attempting 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 are 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.

The second Group (IRG2) is concentrating 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 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 is fabricating novel transformative ion conducting materials by synergistically combining materials with dramatically different ionic transport characteristics.

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. A second class of clathrate structures is the class of metallo-silicon clathrates. Although the structural and electronic properties of these cage-like structures of Si have been studied extensively, little is known about intercalation of methane or hydrogen within the clathrate channels. We have stored up to 1 wt. % of hydrogen in a silicon clathrate material. Recently, we have succeeded in making silicon clathrate materials in larger volumes for our initial experiments in using these materials in solar cells.

In addition to the two research groups, funds were used to support “seed” grants on promising but very preliminary research projects. Six projects funded in 2012 were entitled: s(1) Development of Robust Hybrid Polymer Membranes with Membrane-Protein-Mediated, Light-Driven Proton Transport Performance, (2) Inorganic Clathrates for Renewable Energy Applications, (3) Nonstoichiometric Oxides for Solar Thermochemical Fuels Production, (4) Development of Electrochromic Thin Film Transistors and Dichalcogenides for Sustainable H₂ Production, (5) Quantum Dot Metamaterials, and (6) Electrochemical-Mechanical Force Coupling at Nano- and Micro-Scales in Lithium Intercalation Compounds

Principal Senior Investigators

Funding from CHECRA

P. Craig Taylor, Director	\$25, 000
Reuben Collins, Associate Director and Head IRG1	\$125,000
Andrew Herring, Head IRG2	\$125,000
Carolyn Koh, Head, Seed Grant Program and Head IRG3	\$125,000

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

Center scientists and engineers have succeeded in growing nanometer sized dots and wires of silicon by several different techniques. These techniques include both gas phase growth and liquid solution phase growth. These dots and wires were characterized to analyze their potential for use in solar cell applications. In particular, nanodots of silicon imbedded in an amorphous silicon matrix have shown the most promise for improving the efficiencies of solar cells. For example Center scientists have shown that when electrons are created in the highly absorbing amorphous matrix that they quickly move the crystalline phase where they can be collected much more easily to produce electrical current. Characterization methods have included measuring the optical absorption of light, measuring the electrical conductivity, and characterizing the defects in the various materials. Research on the silicon nanodots imbedded in an amorphous silicon matrix has recently been transferred to another project to be tested in photovoltaic devices.

The transport of ions, such as positively charged hydrogen (protons), in nanostructured films of mixed polymeric and inorganic (oxide) components has been studied to determine the potential use of these films as membranes in fuel cells, batteries, electrolyzers, and other renewable energy devices. This research is focused on the development of nanostructured electrolytes that provide highways for rapid ion transport between the anode and the cathode. The first class of materials is based on polymeric systems derived from monomers molecularly designed to phase segregate into networks of channels that contain water supported by a crystalline matrix. One particular polymer, which is now of great interest to the 3M Company, has higher ionic conductivity and greater stability than any other known polymeric membrane. The second class of membranes includes two-phase nanocomposites produced by introducing nanoparticles into a host matrix. These nanoionic electrolytes manipulate carrier concentration to create interfacial regions with high conductivity. Recently Center scientists have succeeded in making the first ionic transistor that is compatible with standard microelectronic processing procedures. In addition, disparate materials (polymers, metals, and ceramics) have been employed in order to achieve performance that is unattainable with homogeneous systems. Specific targets include increased conductivity, improved stability, and expanded operating windows with respect to temperature and hydration. Center scientists have also made progress on membranes for use in smart window applications. The characterization methods mentioned above have also been employed to study the membrane materials.

Center scientists have been able to produce large quantities (grams as opposed to milligrams) of an open cage (clathrate) structure that is made from silicon. Originally, these clathrate silicon materials were being used to test how much hydrogen could be stored and how easily it could be extracted. Currently Center members are making larger samples of silicon and silicon-germanium clathrates and testing them as materials for solar cell applications. In particular theoretical calculations indicate that these forms of silicon and silicon-germanium exhibit direct optical band gaps, which means that they absorb light much better than the diamond silicon structure that is commonly in use for today's solar cells.

Publications in 2012:

Solar Cell Materials – No CHECRA Support

1. H. Li, **M.T. Lusk**, **R.T. Collins**, **Z. Wu**, "Optimal Size Regime for Oxidation-Resistant Silicon Quantum Dots," ACS Nano 6, 9690-9699, 2012.
2. B.J. Simonds, A. Subramaniyan, **R. O'Hayre**, **P. Craig Taylor**, "Conduction electron resonance used to determine size of palladium nanoparticles in proton conducting ceramics," Journal of Magnetic Resonance 225, 58-61, 2012.
3. B.J. Simonds, I. Perez-Würfl, Y.-H. So, A.S. Wan, S. McMurray, **P.C. Taylor**, "Phosphorous doping of superlattice silicon quantum dots in silicon dioxide," physica status solidi (c) 9, 1908-1911, 2012.
4. Z. Lin, H. Li, **A. Franceschetti**, **M.T. Lusk**, "Efficient Exciton Transport between Strongly Quantum-Confined Silicon Quantum Dots," ACS Nano 6, 4029-4038, 2012.
5. H. Li, Z. Lin, **Z. Wu**, **M.T. Lusk**, "First principles analysis of the initial oxidation of Si (001) and Si (111) surfaces terminated with H and CH₃," J. Chem. Phys. 136, 064507 1-8, 2012.
7. **D.S. Ginley**, **R.T. Collins**, D. Cahen. "Direct solar energy conversion with photovoltaic devices". In: Ginley D.S., Cahen D., editors. Fundamentals of Materials for Energy and Environmental Sustainability. Cambridge, UK: Cambridge University Press; 2012. p. 216-237.
7. I.E. Anderson, R.A. Shircliff, C. Macauley, D.K. Smith, B.G. Lee, **S. Agarwal**, **P. Stradins**, **R.T. Collins**, "Silanization of Low-Temperature-Plasma Synthesized Silicon Quantum Dots for Production of a Tunable, Stable, Colloidal Solution," J. Phys. Chem. C 116, 3979-3987, 2012.

Solar Cell Materials – Partial CHECRA Support

1. V. Popescu, A. Zunger, "Three-dimensional assemblies of semiconductor quantum dots in a wide-gap matrix providing an intermediate band for absorption," J. Appl. Phys. 112, 114320-114320-114310, 2012.
2. L.D. Carr, **M.T. Lusk**, "Quantum physics: Strongly correlated transport," Nature 491, 681-682, 2012.
3. L. Zhang, Z. Lin, J.-W. Luo, **A. Franceschetti**, "The Birth of a Type-II Nanostructure: Carrier Localization and Optical Properties of Isoelectronically Doped CdSe:Te Nanocrystals," ACS Nano 6, 8325-8334, 2012.

4. X. Zhang, L. Yu, A. Zakutayev, A. Zunger, "Sorting stable vs unstable hypothetical compounds : The case of multi-functional ABX Half-Heusler Filled Tetrahedral structures," *Adv. Funct. Mater.* **22**, 1425-1435, 2012.
5. V. Popescu, A. Zunger, "Extracting E versus k effective band structure from supercell calculations on alloys and impurities," *Phys. Rev. B* **85**, 085201 1-12, 2012.
6. F. Lin, J.F. Cheng, C. Engtrakul, **A.C. Dillon**, D. Nordlund, R.G. Moore, T.C. Weng, **S.K.R. Williams**, **R.M. Richards**, "In situ crystallization of high performing WO₃-based electrochromic materials and the importance for durability and switching kinetics," *J. Mater. Chem.* **22**, 16817-16823, 2012.
7. E.E. Hoover, J.J. Field, D.G. Winters, M.D. Young, E.V. Chandler, J.C. Speirs, J.T. Lapenna, S.M. Kim, S.-y. Ding, R.A. Bartels, J.W. Wang, **J.A. Squier**, "Eliminating the scattering ambiguity in multifocal, multimodal, multiphoton imaging systems," *J. Biophotonics* **5**, 425-436, 2012.
8. J.J. Field, K.E. Sheetz, E.V. Chandler, E.E. Hoover, M.D. Young, D. Shi-you, A.W. Sylvester, D. Kleinfeld, **J.A. Squier**, "Differential Multiphoton Laser Scanning Microscopy," *Selected Topics in Quantum Electronics, IEEE Journal of* **18**, 14-28, 2012.
9. C.G. Allen, D.J. Baker, T.M. Brenner, C.C. Weigand, J.M. Albin, K.X. Steirer, D.C. Olson, C. Ladam, **D.S. Ginley**, **R.T. Collins**, **T.E. Furtak**, "Alkyl surface treatments of planar zinc oxide in hybrid organic/inorganic solar cells," *J. Phys. Chem. C* **116**, 8872-8880, 2012.

Membrane Materials – No CHECRA Support

1. J.S. Fish, C.-P. Li, **J.D. Fehribach**, **C.A. Wolden**, **R. O'Hayre**, **A.L. Bunge**, **C.E. Goodyer**, "Poisson-Boltzmann model of space charge layer effects on conductivity in randomly distributed nanoionic composites," *Electrochim. Acta* **83**, 454-462, 2012.
2. J. Tong, A. Subramaniyan, H. Guthrey, D. Clark, **B.P. Gorman**, **R. O'Hayre**, "Electrical conductivities of nanoionic composite based on yttrium-doped barium zirconate and palladium metal," *Solid State Ionics* **211**, 26-33, 2012.
3. G.J. Schlichting, J.L. Horan, J. Jessop, S. Nelson, S. Seifert, Y. Yang, **A.M. Herring**, "A hybrid organic/inorganic ionomer from the copolymerization of vinyl phosphonic acid and zirconium vinyl phosphonate," *Macromolecules* **45**, 3874-3882, 2012.
4. C.-P. Li, **C.A. Wolden**, **A.C. Dillon**, **R.C. Tenent**, "Electrochromic films produced by ultrasonic spray deposition of tungsten oxide nanoparticles," *Solar Energy Mater. Solar Cells* **99**, 50-55, 2012.

5. C.-P. Li, **R.C. Tenent**, **A.C. Dillon**, R.M. Morrish, **C.A. Wolden**, "Improved Durability of WO₃ Nanocomposite Films Using Atomic Layer and Vapor Deposited Coatings," *ECS Electrochem. Lett.* **1**, H24-H27, 2012.
6. W. Lee, F.B. Prinz, X. Chen, S. Nonnenmann, D.A. Bonnell, **R.P. O'Hayre**, "Nanoscale impedance and complex properties in energy-related systems," *MRS Bull.* **37**, 659-667, 2012.
7. **C.E. Goodyer**, **A.L. Bunge**, "Mass transfer through membranes with surface roughness," *J. Membrane Sci.* **409-410**, 127-136, 2012.
8. J.R. Ferrell, S. Sachdeva, T.A. Strobel, G. Gopalakrishan, **C.A. Koh**, G. Pez, A.C. Cooper, **A.M. Herring**, "Exploring the fuel limits of direct oxidation proton exchange membrane fuel cells with platinum based electrocatalysts," *J. Electrochem. Soc.* **159**, B371-B377, 2012.
9. A.M. Deml, **A.L. Bunge**, M.A. Reznikov, A. Kolessov, **R.P. O'Hayre**, "Progress toward a solid-state ionic field effect transistor," *J. Appl. Phys.* **111**, 074511, 2012.

Membrane Materials – Partial CHECRA Support

1. Y. Liu, J.L. Horan, G.J. Schlichting, B.R. Caire, M.W. Liberatore, S.J. Hamrock, G.M. Haugen, M.A. Yandrasits, S. Seifert, **A.M. Herring**, "A Small-Angle X-ray Scattering Study of the Development of Morphology in Films Formed from the 3M Perfluorinated Sulfonic Acid Ionomer," *Macromolecules* **45**, 7405-7503, 2012.
2. **A.M. Herring**, J.L. Horan, M.-C. Kuo, J.D. Jessop, G.J. Schlichting, Y. Yang, "Advanced hybrid super acidic inorganic-organic PEMs for hotter and drier operation," *Proceedings of Polymer Electrolyte Fuel Cells 12*, in press, 2012.
3. F. Lin, C.-P. Li, G. Chen, **R.C. Tenent**, **C.A. Wolden**, D.T. Gillaspie, **A.C. Dillon**, R.M. Richards, C. Entrakul, "Low-temperature ozone exposure technique to modulate the stoichiometry of WO_x nanorods and optimize the electrochromic performance," *Nanotechnology* **23**, 255601 1-8, 2012.
4. F. Lin, J.F. Cheng, C. Entrakul, **A.C. Dillon**, D. Nordlund, R.G. Moore, T.C. Weng, **S.K.R. Williams**, **R.M. Richards**, "In situ crystallization of high performing WO₃-based electrochromic materials and the importance for durability and switching kinetics," *J. Mater. Chem.* **22**, 16817-16823, 2012.

Seed Funding– No CHECRA Support

1. A.M. Deml, **A.L. Bunge**, M.A. Reznikov, A. Kolessov, **R.P. O'Hayre**, "Progress toward a solid-state ionic field effect transistor," *J. Appl. Phys.* **111**, 074511, 2012.

Seed Funding– Partial CHECRA Support

1. R.G. Grim, P.B. Kerkar, M. Shebowich, M. Arias, E.D. Sloan, **C.A. Koh**, A.K. Sum, "Synthesis and Characterization of sI Clathrate Hydrates Containing Hydrogen," J. Phys. Chem. C **116**, 18557-18563, 2012.

Education and Outreach – Partial CHECRA Support

None

Attachment B

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)

Reporting Period: January 1-December 31, 2012

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. Jörg E. Drewes, is a collaborative effort among four research universities in the West, 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, we will advance tools like life-cycle assessment for decision-making and conduct 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. 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.

At CSM, the *Efficient Engineered Systems* thrust will be supported by two research groups (E1 and E2). Research group E1 develops engineered solution to facilitate reuse of municipal wastewater effluent tailored to local needs. The engineered solutions will be part of a smart urban water grid where distributed treatment systems facilitate water reuse while minimizing the overall energy and carbon footprint. These approaches require the design and operation of highly flexible treatment systems that are remotely monitored and supervised. A high degree of flexibility is needed since water reuse needs can change as a function of season and location. Treatment systems developed and tested under E1 are using hybrid technologies using sequencing batch reactors coupled with membrane bioreactor processes. Selective desalination processes, such as electrodialysis reversal, are employed to remove certain salts that limit certain reuse applications. In addition, research group E2 will focus on treatment processes that enable the recover of energy contained in wastewater streams through modified anaerobic processes and use of microalgae. These efforts are supported through close collaborations with industry partners and start-up companies in Colorado.

Throughout the 19th and 20th centuries, natural aquatic systems had an uneasy coexistence with water infrastructure. As urban population increased, engineered structures replaced natural aquatic systems as surface waters were routed to storm sewers and urban hydrology was altered by impermeable surfaces reducing groundwater infiltration. During the latter half of the 20th century, recognition of the adverse impacts on aquatic systems from the discharge of wastes and modification of urban hydrology led to the passage of the Clean Water Act and Federal Bonds to support the construction of treatment systems to protect aquatic ecosystems. While this

approach resulted in dramatic improvements in water quality, water managers are increasingly cognizant of its limitations and have begun to advocate for the integration of natural systems into urban water infrastructure as a means of enhancing water quality, improving system resiliency, and reducing energy consumption while simultaneously preserving ecosystem integrity and providing aesthetic benefits. Unfortunately, natural systems are complex, and our understanding about how to actively manage them as part of urban water infrastructure is limited. As a result, water managers are uncertain about how to invest in projects involving managed natural systems. Furthermore, our failure to understand how natural systems respond to active management prevents us from fully realizing the potential benefits they can provide with respect to water storage and the improvement of water quality.

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 research is led by three research groups with the goals to: (i) develop tools for manipulating natural systems to enhance water quality (N1); (ii) integrate managed aquifer recharge into urban settings using reclaimed water leading to drinking water augmentation (N3); and (iv) harvest stormwater and infiltrate in urban settings to augment local supplies (N4).

Within the Urban Systems Integration and Institutions thrust, research group U1 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, twelve projects were funded in 2012 and are entitled:

- Integrated Regional Economic-Hydraulic Models (U1.1);
- Tools to support decision making for nested, spatially-scaled, integrated urban water infrastructure (U1.2);
- Tailored water for distributed non-potable reuse using sequencing batch/membrane bioreactor hybrid systems (E1.1);
- Sustainable landscape irrigation with reclaimed water (E1.3);
- Point-of-entry water treatment for potable reuse (E1.4);
- Microalgae for wastewater treatment and recovery: A new approach to onsite wastewater treatment (E2.2);
- Anaerobic digestion as primary treatment at WWTPs (E2.4);
- Design of unit process wetlands to optimize chemical contaminant removal (N1.2);
- Hyporheic zone management for water quality improvement (N2.3);

- Managed aquifer recharge and recovery: Simulation, modeling and operation (N3.1);
- Aquifer storage, treatment, and harvesting of stormwater for distributed reuse: coupled modeling, laboratory and field studies (N4.1); and
- Methodologies, models, and materials for predictable removal of chemicals from stormwater during distributed recharge (N4.3).

Principal Investigators

Funding from CHECRA

Jörg E. Drewes, Research Director and	\$42,297
Project Co-Lead Tailored Water, E1.1	\$22,790
Project Lead Point-of-Entry Treatment, E1.4	\$37,867
Tzahi Cath, Engineered System Thrust Leader and	
Project Lead Decision Support Tools, U1.2	\$10,838
Project Co-Lead Tailored Water, E1.1	\$22,790
Project Lead Microalgae Wastewater Treatment, E2.2	\$1,851
Linda Figueroa, Project Lead Anaerobic Digestion, E2.4	\$7,827
Christopher Higgins, Project Lead Subsurface Purification, N4.3	\$23,009
John McCray, Project Lead Hyporheic Management, N2.3	\$12,921
Reed Maxwell, Theme Leader Modeling Complex Systems and	
Project Lead Managing Complex Urban Water, U1.1	\$90,502
Project Lead Coupled Modeling, N4.1	\$28,945
Barbara Moskal, Education Lead	\$0
(funds in 2012 were from NSF and CSM)	
Junko Munakata-Marr, Project Lead Sustainable Irrigation, E1.3	\$16,283
Jonathan Sharp, Project Lead Unit Process Wetland, N1.2	\$5,446
Kathleen Smits, Project Lead Aquifer Management, N3.1	\$22,257
 TOTAL Spending (Jan-Dec 2012)	 \$345,623

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

Jörg E. Drewes: Discretionary funding for supporting new research directions; design and installation of new testing apparatus; travel support for students and faculty; and student support. Funding for one graduate student who conducted an energy audit of a decentralized hybrid water reclamation facility facilitating local tailored non-potable reuse (E1.1) and one graduate student who is developing a prototype using ceramic nanofiltration membrane coupled with UV oxidation for point-of-entry drinking water treatment (E1.4). Partial salary support for one postdoctoral research associate to manage the full-scale sequencing batch reactor with submerged ultrafiltration membrane bioreactor (SBMBR) (E1.1). Nominal funding was also used for materials and supplies for SBMBR operation (E1.1).

Tzahi Cath: Partial salary support for an Assistant Research Faculty member to develop a decision support tool to aid tailoring water treatment for specific beneficial use (U1.2). Funding used to cover materials and supplies for bench scale testing of nutrient and energy recovery from wastewater using specific target microalgae (E2.2).

Linda Figueroa: 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).

Christopher Higgins: Funding for one graduate student who is developing special adsorbants to remove chemical contaminants in stormwater during distributed recharge (N4.3). Funding also provided for materials and supplies in support of chemical analysis using liquid chromatography tandem mass spectrometry (LC-MS/MS).

John McCray: Partial funding for one postdoctoral research associate and one hourly graduate student to study water quality improvements in the hyporheic zone to develop management strategies for urban stream restoration (N2.3).

Reed Maxwell: Salary support for one postdoctoral research associate and one graduate student who spearheaded initial hydrological modeling efforts for modeling case study in close collaboration with Aurora Water, CO (U1.1). Funding for a second postdoctoral research associate who develops watershed-scale models to locate distributed stormwater recharge facilities (N4.1). This study is currently focusing on the Cherry Creek water shed in Denver.

Junko Munakata-Marr: Funding for one graduate student and one hourly undergraduate graduate student for the establishment of test cells for soil treatment of irrigated reclaimed water (E1.3). Nominal funding for materials and supplies needed for monitoring of the test cells.

Jonathan Sharp: Funding to cover supplies and materials to study the biocommunity diversity in unit processes wetlands to better understand key boundary conditions for the attenuation of trace organic chemicals (N1.2).

Kathleen Smits: Funding for one graduate student who designed and constructed a 3-D intermediate-scale tank experiment to simulate fate and transport processes of artificial recharge and recovery facilities (N3.1). Partial summer salary was also provided to the new Assistant Professor in support of early career development.

Results achieved

Center scientists and engineers have established a research test bed on the Colorado School of Mines campus that utilizes and treats municipal wastewater (~7,000 gal/day) in a demonstration-scale treatment unit to tailor effluent qualities to various reuse applications (i.e., urban landscape irrigation; toilet flushing; streamflow augmentation; groundwater recharge) (E1). This effort is supported through collaborations with

manufacturers and start-up companies within Colorado. After an initial period of testing demonstrating proof-of-concept, center scientists have investigated optimization strategies to generate on-demand effluent qualities with elevated levels of nitrogen while simultaneously optimizing energy demands. In addition, researchers demonstrated through state-of-the-art genomic studies that this operational regime from a microbial standpoint is highly robust.

Activities within the natural water infrastructure systems thrust revealed dependencies between organic carbon and nutrient levels for the establishment of a microbial community in artificial recharge and recovery facilities as well as wetland cells that are the determining factors for enhancing the removal of trace organic chemicals. Advanced metagenomic tools are now used in conjunction with state-of-the-art chemical characterization techniques to better characterize the underlying processes with the goal to develop predictive strategies regarding operation and finished water quality.

Center scientists within the U1 research group have developed a conceptual model that couples supply options with demand while also considering water treatment/distribution as well as wastewater collection and treatment. This model will be tailored to serve as regional model for major water utilities, such as Aurora Water, to investigate how utilities might deploy technologies, strategies, and policies in order to increase overall efficiency of water and energy use. The model will also allow characterizing inefficiencies in the current system. The model is based on a flexible, module-based simulation framework.

Publications and Presentations in 2012:

Journal Papers and Book Chapter:

- Bischel, H.N., Lawrence, J.E., Halaburka, B.J., Plumlee, M.H., Bawazir, A.S., King, J.P., McCray, J.E., Resh, V.H., Luthy, R.G. (2013). Renewing urban streams with recycled water for streamflow augmentation: Hydrologic, water quality, and ecosystem services management. *Environmental Engineering Science*, in press.
- Forrestal, C., Xu, P., Ren, Z. (2012). Sustainable desalination using a microbial capacitive desalination cell. *Energy & Environmental Science*, doi: 10.1039/C2EE03956F.
- Hancock, N.T., Xu, P., Heil, D.M., Bellona, C., and Cath, T.Y. (2011). Comprehensive bench- and pilot-scale investigation of trace organic compounds rejection by forward osmosis. *Environmental Science and Technology*. 45 (19): 8483-8490. doi: 10.1021/es201654k.
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- Higgins, C.P. "Accumulation of Emerging Contaminants in Foodcrops from Reclaimed Water and Biosolids- Amended Soils" Association of Analytical Communities 126th Annual Meeting and Exposition, 30 September – 3 October, 2012. Las Vegas, Nevada.
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APPENDIX C

Liquid Crystal Materials Research Center

University of Colorado – Boulder

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

Summary: The Liquid Crystal Materials Research Center (LCMRC or the Center) has existed on the University of Colorado – Boulder campus since the early 1980s, with block funding from the NSF Division of Materials Research since September 1998. The LCMRC is currently funded as an NSF Materials Research Science and Engineering Center (MRSEC), one of an elite national network of advanced materials research programs.

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

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

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

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

In 2012, the CHECRA funding was allocated to the three focus areas of the center described in this summary – research, industrial outreach, and education outreach (in particular industrial and K-12 outreach).

FUNDING ALLOCATED TO EACH PRINCIPAL PERSON OR ENTITY

Research - The past year of MRSEC, with NSF funding supplemented by the CHECRA matching state funds, has continued in its role as CU Boulder's single most visible materials research group nationally

and internationally. Highlights of CHECRA funding published in the most prestigious journals, include discovery of a new polar smectic phase of bent-core molecules, appearing in *Science*, observation of a photo-addressable self assembled monolayer system for alignment of liquid crystals, appearing in *Nature Communications*, and development of fundamental new insights into the topology of defects and textures in liquid crystals and polymers, appearing in *Nature*.

Non-contact optical manipulation is typically achieved by use of forces and torques exerted by tightly focused laser beams and has been instrumental for many scientific breakthroughs. However, non-contact optical manipulation finds rather few technological applications because of the small-area manipulation restrictions, the needed high laser powers, and complexity of implementation. Recent efforts in the LCMRC have been directed toward extending the scope of non-contact optical control through the use of optically-guided electrokinetic forces, vortex laser beams, and plasmonics, applications of which, however, are very limited when suspending fluids are liquid crystals. Center researchers have demonstrated an approach for large-area manipulation of colloidal nano- and microparticles and their self-assembled superstructures in LC anisotropic fluids by means of single-molecule-thick, light-controlled surface monolayers. Using light of intensity from 1000 to 100,000 times smaller than that in conventional optical tweezers, we have rotated, translated, localized, and assembled particles of various sizes, shapes, and compositions suspended within a LC host on the monolayer.

Photosensitive derivitized methyl red (dMR) monolayers, which have been developed in the LCMRC for their liquid crystal alignment properties, could lead to a wide range of additional applications for light-controlled command surfaces. When exposed to polarized light, the monolayers rapidly display an anisotropic anchoring energy with unprecedented sensitivity. We are working to understand the nature of this high sensitivity, as well as the origin of additional characteristics of these layers. In the future we will continue to explore a variety of photoactive command surfaces that enable light-driven modification of the surface energy, including its orientation dependence. These systems will be based on azobenzene containing small molecules attached through silane chemistries, as well as acid-base bonding and peptide "click chemistries". Our objectives will be to establish spatially variable (patterned) alignment of single-phase liquid crystal media as well as photo-control of wetting, boundary layer lubrication and phase transitions. We will explore both smooth and nanostructured surfaces, such as those involving inorganic nanowire arrays. These layers will be studied with surface-sensitive vibrational spectroscopies: resonant sum-frequency generation, surface enhanced Raman scattering, and FTIR ellipsometry.

Suspensions of graphene oxide sheets in water exhibit stripe textures spontaneously at concentrations large enough to give a liquid crystal phase. Nearly identical textures are found in systems of disc-shaped clay particles. These textures cannot be understood on the basis of standard liquid crystal elasticity and have led us to the notion of flexopolydispersity which is liquid crystal elasticity incorporating the effects that arise because the material under consideration is not a neat material but a suspension that can vary spatially both in concentration and composition of constituent particles. Such variations have been shown to have distinct consequences for the phase behavior of suspensions of anisometric particles and we have found that elasticity is also affected. Basic flexopolydispersive effects in polydisperse suspensions of discs are the segregation of smaller area discs to regions of high curvature, depletion of discs from the core region of topological defects, and depletion interactions stabilizing such structures. Understanding

such textures is critical for taking advantage of the many new potential applications of such layered materials.

The LCMRC has developed single-molecule total internal reflection fluorescence microscopy methods and applied these methods to study dynamic molecular behavior of surfactants, proteins, and nucleic acids at the solid-liquid, liquid-liquid, and nematic-liquid interfaces. The group has also explored phenomena that involve recognition of double-stranded DNA using nematic liquid crystals, with the ultimate goal of developing LC-based DNA microarray technologies. In one approach, DNA hybridization at the nematic-aqueous interface in the presence of a cationic surfactant causes a reorientation of the LC material from tilted to homeotropic anchoring. Recent studies of DNA-surfactant interactions at the nematic-aqueous interface have led to an improved understanding of the interplay between cooperative and competitive adsorption of these two species. These experiments are being pursued in an effort to improve the sensitivity and specificity of this approach. Another approach involves azimuthal alignment of nematic LCs by extended ssDNA and dsDNA molecules on a surface that otherwise imparted a negligible influence on LC orientation. As expected, single-stranded DNA led to LC orientation in the direction of extension. However, extended double-stranded DNA (dsDNA) molecules caused LC alignment at angles oblique to the extension direction, providing a unique characteristic response to the chiral dsDNA helix that was readily observed using polarized light. The intrinsic amplification effect due to LC orientational correlations enabled direct observation of a signal from a single molecule of extended dsDNA.

Polymerized lyotropic (i.e., amphiphilic or surfactant) LC (LLC) materials have recently garnered both fundamental and applied interest because their stabilized, ordered, nanoporous structures can be used as unique nanoenvironments for heterogeneous catalysis, molecular size separations (membranes), and enhanced transport. Typically, LLC assemblies and their polymerizable analogues are formed around water as the hydrophilic liquid component in the amphiphilic self-organization process. Only a handful of examples of LLC systems are known that can form around non-aqueous solvents as a water substitute (ethylene glycol, glycerol, formamide, N-methylformamide, dimethylformamide, N-methylsyringone, and some imidazolium-based room-temperature ionic liquids (RTILs), which are molten organic salts at ambient temperature). From a fundamental scientific point of view, such non-aqueous LLC systems are interesting because they represent new interfacial and ordering phenomena in amphiphilic systems on the nanoscale. From an applied perspective, non-aqueous LLC and LLC polymer systems provide entry points into nanoscale reaction and transport chemistry and phenomena that are not reliant or dependent upon water. We have pioneered an unprecedented, non-aqueous, polymerizable LLC system based on a monomer that forms a bicontinuous cubic LLC phase with 3-D interconnected nanopores around the common liquid electrolyte solvent, propylene glycol (PC) and its salt solutions.

The B4 liquid crystal phase is perhaps the most complex and unique soft materials system known. While the basic story around the structure of B4, as described by the LCMRC in 2009, is understood, some key questions remain outstanding, including whether B4 is limited to benzylideneanilines. Synthesis and characterization of a new structural class of B4 materials, the W513 series, reveals the B4 phase in a different chemical family. All seven homologues in this series exhibit the B4 phase, and FFTEM imaging of these homologues will allow estimation of the helical nanofilament (HNF) pitch and diameter as a function of tail length.

We also pursue the macroscopic alignment of the helical nanofilament phase. The HNF phase is fluid at temperatures close to where in forms from the isotropic, and in this regime can be aligned by shear flow quite well. We put the LC in micron-size channels on a surface to hold it in place while air flow over the surface does the alignment. Anticipated organic photovoltaic applications will require alignment with the filaments normal to planar substrates, a topic of ongoing research.

Industrial Outreach - The Colorado high tech industry community continues to benefit from the Center. Center graduate students and postdocs have taken jobs in several local companies, including the R&D group at RealD, which recently gained recognition for providing the technical underpinnings of the modern 3D movies, including Avatar. A Center graduate (Chair of the Center Technology Advisory Board) is working in Boulder County in the R&D group for Serious Materials, with the goal of improving on the Serious Materials world-class energy efficient windows.

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, and dedicated to commercialization of FLCs, was recently acquired by Micron Technology, Inc., headquartered in Idaho. The Displaytech team continues to work in their labs and offices in Longmont, and continues to expand their business around a line of sophisticated display engines. The same device is being applied by Light Blue Optics, with headquarters in Cambridge, England, and offices in Colorado Springs, in a completely new kind of projector technology where the image is a two-dimensional hologram. These projectors are scheduled to become commercial in the immediate future.

Center researcher David Walba has recently become an Associated Researcher at the National Renewable Energy Laboratory, working on liquid crystal composites for organic photovoltaic devices. This project, which developed as a result of a Center sponsored LCOPV workshop, aims to evaluate the electrical and photoresponse characteristics of the Center's helical nanofilament (HNF) phases for organic photovoltaic applications. Initial experiments, in which the photogenerated carrier lifetimes in HNF structures doped with C60 homolog PCBM have proven to be exceptionally exciting, with these composites exhibiting extremely long carrier lifetimes.

Education Outreach - Highlights from the past year include expansion of the *Materials Science from CU* program, now one of CU's most effective K-12 outreach programs. In outreach to children (and parents), the focused attention of a dedicated outreach Director has enabled many notable successes over the past year. Examples include:

Materials Science from CU delivered 70 classes to 2,800 Colorado children, bringing Center personnel into the classroom using the understanding of materials to teach physical science concepts (1,830 classes to 75,000 students over the past 11 years).

Center senior investigator participated in a variety of high school and undergraduate research experience and undergraduate/graduate minority access programs in 2012.

The LCMRC NSF Partnership for Research and Education in Materials (PREM) funding for support of undergraduate and graduate research opportunities now has two of its minority undergraduate students now pursuing Ph.D.s in the Center.

Appendix D

CHECRA Report for 2012

Engineering Research Center in Extreme Ultraviolet Science and Technology

Colorado State University

University of Colorado

Director: Prof. Jorge J. Rocca. Colorado State University

Deputy Director: Prof. Margaret M. Murnane. University of Colorado

CHECRA Grant: \$200,000 (2008, 2009), \$400,000 (2010-2013)

Project Summary

The National Science Foundation (NSF)-funded Extreme Ultraviolet Science and Technology Engineering Research Center, a partnership between Colorado State University and the University of Colorado, is a world leader in the generation and application of light beyond the ultraviolet to challenging scientific and industrial problems that include nanotechnology, advanced materials, clean energy, and in the near future biology. The Center was supported by \$ 2.67 Million from NSF core funding in 2012, for a total of \$ 35.96 Million in core NSF funding since its inauguration in 2003. The funding provided by the Colorado Higher Education Competitive Research Authority (CHECRA) was crucial in assisting the Center to achieve renewal by the National Science Foundation in 2010, which extended funding by NSF until October 2013 with a possible no-cost extension until March 2014. It also contributed to the Center's ability to obtaining funding from other Federal agencies, amounting to \$ 3.8 Million for 2012. During 2012 the Center also received \$ 0.257 Million in industry funding. The Center is making important contributions to the research output, education, industrial and economical health of the state.

Description of the project, the principal persons or entities involved in the project

Light in the Extreme Ultraviolet (EUV) region of the spectrum (wavelengths approximately 1 to 50 nm) has become a critical enabling technology in areas of great importance to the national economy, as the size of the most advanced electronic circuits and nanoscale machines continues to shrink below the wavelength of visible light. Furthermore, exciting new opportunities in science arise from the possibility of focusing EUV light to unprecedented small spot sizes, short pulse durations, and extremely high intensities. Further development of EUV technologies will open up a variety of new areas of investigation, including new tabletop probes of surface, chemical, cellular samples, nanostructures and materials, and the development of a new generation of nanoprobe. In response to these challenges and opportunities, in October 2003 NSF funded the ERC in Extreme Ultraviolet Science and Technology.

The Center combines the complementary expertise of Colorado State University and the University of Colorado—leaders in compact EUV light sources and applications—with a set of partner institutions that include the University of California Berkeley/Lawrence Berkeley National Laboratory and four year Colleges, other universities, national laboratories, and a set of sixteen industrial corporate members. At Colorado State University Center the faculty includes Profs. Jorge Rocca, Carmen Menoni, Mario Marconi, and Elliot Bernstein with affiliations to the

Electrical Engineering, Chemistry and Physics departments. At the University of Colorado the Center Faculty includes Profs. Margaret Murnane, Henry Kapteyn and Rongui Yang, with affiliations to the Physics Department, JILA, the Electrical and Computer Engineering and Mechanical Engineering Departments.

To realize the full impact of EUV technology in manufacturing and in scientific research we are developing a new generation of compact coherent EUV sources with unique capabilities and we are combining them with advanced EUV optics to implement engineered systems designed to solve challenging engineering and scientific problems. Breakthroughs in new EUV lasers and in High Harmonic Generation sources have significantly expanded their spectral coverage, in some cases increasing the average power by orders of magnitude. In the past year we have made significant advances in the development of compact high brightness coherent EUV and soft x-ray sources and have broken new ground and established new records in integrating them into engineered systems. By integrating the new compact sources with advanced EUV optics, we have developed a new set of microscopes, materials modification stations, and spectrometers with unique capabilities for a broad range of applications in industry and science. These include compact EUV microscopes with sub-38 nm resolution, a laser ablation testbed capable of producing sub-100 nm holes, an EUV photoacoustic metrology testbed to characterize thin films, a lensless microscope with 20 nm spatial resolution and elemental sensitivity, a single photon ionization spectrometer for the study of nanoclusters, a table-top workstation for the patterning of arrays of nanostructures;

This Center makes an important contribution to education in Colorado, ranging from graduate education and undergraduate education to elementary school. We are addressing the shortage of engineers and scientist with expertise in EUV technology by training a large number of students and young scientists, several of which have now graduated and joined industries in Colorado. Our Research Experience for Undergraduate program (summer and year-round) has already mentored 195 students, with a significant fraction of the summer participants from under-represented minority groups. During 2011 the Center received \$ 287,000 of additional funding from NSF to establish and REU site, to provide research experiences for undergraduates during 2012-2014. We have also developed a successful set of workshops for K-12 students and teachers. The Center supports High School student researcher internships during the summers, and also has a program in which Middle School teachers spend part of the summer conducting research at the Center and developing material they can take back to the classroom. Optics teaching kits containing materials and curriculum for standards-based hands-on activities were distributed to over 100 K-12 teachers. In 2012 we again held the annual "Optics After School" Lab program for High School Students. This 5 day event has enrolled the participation of 163 High School students since the Center started. To further ensure the active participation of under-represented groups, the Center is working with the Colorado Louis Stokes Alliance for Minority Participation at CSU, the Science Discovery Program at CU-Boulder.

The 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 \$400K in state matching funds to the Center for 2012 were distributed in equal parts among Colorado State University and the University of Colorado to support graduate students and

young scientists who worked in collaboration at Colorado State University and at the University of Colorado to develop new sources and applications of EUV laser light

At Colorado State University, the CHECRA matching funds for the NSF EUV ERC were used to support a post-doctoral student and two young research scientists. They worked in close collaboration with graduate and undergraduate students and the PI in the development of new EUV laser light sources, and to employ these laser sources in the development of new techniques to pattern arrays of nano-structures and to map the composition of samples both organic and inorganic samples in three-dimensions with nanoscale resolution. During 2012 the average power and repetition rate of these compact lasers were increased by nearly an order of magnitude, establishing world records for table-top EUV lasers. The coherence and high average flux EUV beams produced by these lasers were used to demonstrate error-free printing of nano-scale patterns, and to directly machine nano-scale-features as described in the publications below. Efforts in nano-scale imaging also continued with the publication of the first table-top demonstration of the recording of a movie of nano-phenomena. Finally, progress was made in the development of a new type of analytic laser probe that using the superior spatial resolution of focused EUV laser light to map the composition of materials with nano-scale resolution.

The University of Colorado used their \$ 200K State Matching funds for the NSF EUV ERC to support two postdoctoral researchers. These young scientists worked on key technologies of the Center – the development of compact laser and x-ray sources with wavelengths less than 1 nanometer, and also the development of new microscopy and nanometrology techniques. A major advance occurred in 2012, with the publication of laser-like beams up to photon energies of 1keV, which are of interest for imaging at the nanoscale with elemental and chemical sensitivity. Many applications of these technologies are being implemented in collaboration with NIST Boulder Labs, industry and other collaborators including: the development of new microscopes capable of high-resolution nanoimaging of thick materials samples; characterization of interfaces and thin films of interest to the semiconductor and data storage industries; measurements of heat transport in nanostructures of interest to electronics and photovoltaics; and understanding and optimizing magnetic materials on nanoscale dimensions for applications in data storage. [see references] Past work on laser and x-ray sources has already been commercialized and has led to a 38-person spin-off company in Boulder. [KMLabs link:www.kmlabs.com.] The current work on new coherent x-ray sources and advanced microscopes will also be commercialized in the future.

Summary to Benefits to the State of Colorado

- In 2012 the Center received \$2,670,000 for core funding from the NSF.
- On top of this NSF core funding, the Center generated \$ 3.8 M in funding from Federal Agencies during 2012 for Colorado State University and University of Colorado.
- The Attracted \$ 257,000 in funding from industry during 2012, of which \$200,000 were in cash
- Supported ~ 50 graduate and undergraduate students and faculty in Colorado;
- Graduated numerous students with PhD or MS degrees who were hired by Colorado high technology companies (e.g. Brooks Automation, KM Laboratories, InPhase, Avago);

- Assisted Colorado companies in bringing new products to the market (e.g., Precision Photonics, KM laboratories);
- Provides research experiences for undergraduate students (22 students during 2012)
- Reached 880 K-12 students and 72 teachers with science workshops and demonstrations during 2012.
- Continued to provide summer research experiences for middle school teachers and high school students
- Research experiences for high school students (7 Colorado high school students during 2012).
- Research experiences of high school teachers (20 teachers during the duration of the program, 2 teachers during 2012)
- Increases the National and International reputation of Colorado as a leader in advanced technology and science. Major awards to Center faculty during 2012 are listed below.

Major Center faculty awards for 2012

Profs. Henry Kapteyn, Margaret Murnane, and Jorge Rocca shared the 2012 Willis Lamb Prize for Laser Science and Quantum Optics. <http://www.lambaward.org/>

Center Peer Review Journal Publications for 2012

1. B. A. Reagan, K. A. Wernsing, A. H. Curtis, F. J. Furch, B. M. Luther, D. Patel, C. S. Menoni, J. J. Rocca, "Demonstration of a 100-Hz repetition rate gain-saturated diode-pumped table-top soft x-ray laser," *Optics Letters*, **37**, 3624 (2012).
2. L. Urbanski, M.C. Marconi, L.M. Meng, M. Berrill, O. Guilbaud, A. Klisnick, and J.J. Rocca, "Spectral linewidth of a Ne-like Ar capillary discharge soft-x-ray laser and its dependence on amplification beyond gain saturation", *Physical Review A*, **85**, 033837 (2012)
3. L. Urbanski, A. Isoyan, A. Stein, J. J. Rocca, C. S. Menoni, M. C. Marconi, "Defect-tolerant extreme ultraviolet nanoscale printing," *Optics Letters*, **37** (17), 3633 (2012).
4. S. Carbajo, I. D. Howlett, F. Brizuela, K. S. Buchanan, M. C. Marconi, W. Chao, E. H. Anderson, I. Artioukov, A. Vinogradov, J. J. Rocca, and C. S. Menoni, "Sequential single-shot imaging of nanoscale dynamic interactions with a table-top soft x-ray laser", *Optics Letters*, **37** (14), 2994 (2012)
5. L. Urbanski, W. Li, J. J. Rocca, C. S. Menoni, M. C. Marconi, A. Isoyan, and A. Stein, "Defect tolerant extreme ultraviolet lithography technique," *J. Vacuum Sci. and Tech. B*, **30**, 06F502 (2012).
6. B. A. Reagan, A. H. Curtis, K. A. Wernsing, F. J. Furch, B. M. Luther, and J. J. Rocca, "Development of high energy diode-pumped thick-disk Yb:YAG chirped-pulse-amplification lasers," *IEEE J. Quantum Electronics*, **48**, 827, (2012) (invited)

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Attachment E

Center for Multiscale Modeling of Atmospheric Processes (CMMAP)

Colorado State University

Principal Senior Investigators:

Director: David A. Randall, Colorado State University

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

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

Director of Knowledge Transfer: Steve Krueger, University of Utah

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

Funding from CHECRA

CHECRA Grant: \$150,000 per year, total of five years, CSU Fiscal years 2012-2016, total of \$750,000

Summary: CMMAP is one of seventeen current NSF-sponsored Science and Technology Centers. CMMAP is a partnership of research and educational institutions, government agencies, and industry. The Center is currently in its “sustainability” phase and is focusing its research on improving the representation of cloud processes in climate models. The need for such improvements is one of the most important limitations on the accuracy of current climate-change simulations. CMMAP is addressing this problem 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 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 by disseminating teaching materials to K-12 teachers and the State of Colorado Governor’s Energy Office. CHECRA funding is being distributed to all three of the focus areas of the Center.

Description of the project, the principal persons or entities involved in the project

Cloud processes are central to the Earth Sciences. Changes in cloudiness can either amplify or damp climate change. Clouds are a key element 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 predict global cloudiness.

The Center for Multiscale Modeling of Atmospheric Processes (CMMAP) is focused on improving the representation of cloud processes in climate models. The need for such

improvements has been one of the most important limitations on the reliability of climate-change simulations. Over the past several decades, progress towards improved predictions of the effects of clouds on weather and climate has been unacceptably slow. *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.*

CMMAP's research and knowledge-transfer (RKT) goals are to drastically improve the representation of cloud processes in global atmospheric models through the explicit representation of cloud processes on fine grids, accomplished through various computational strategies including the multi-scale modeling framework (MMF) and global cloud-resolving models. Today, many of the world's major modeling centers are moving quickly to develop such capabilities. CMMAP is a Center, not a project, in part because it brings together scientists from a broad range of disciplines at dozens of institutions to work towards this common goal. The team includes climate modelers, cloud modelers, and experts on turbulence, radiation, cloud physics, and observations. The end results include improved understanding of important climate phenomena, such as the Madden-Julian Oscillation and cloud feedbacks on climate change.

In addition, however, CMMAP is a Center because, like all STCs, its mission goes far beyond research. CMMAP devotes enormous amounts of time and energy to its Education and Diversity (ED) components. With the perspective that comes from almost five years of nurturing the Center, we can see that CMMAP's ED mission is highly complementary to its RKT mission. We have vertical integration within our RKT and ED stovepipes, but we also have horizontal integration between RKT and ED. Our ED activities make our RKT activities work better, and vice versa. The interdisciplinary collaborations within the Center allow us to accomplish more than ED or RKT could do separately.

CMMAP's students, teachers, and researchers fit together comfortably and productively as a team. The broad spectrum of CMMAP's activities has made the Center into a true collaborative community, populated by a variety of people with a range of interests, skills, goals, and ages, working together to help each other succeed. CMMAP integrates atmospheric scientists, writers, sociologists, computer scientists, policy analysts, educational psychologists, and others, who work together towards common goals whose value and importance we collectively acknowledge and appreciate. CMMAP has a culture. It is much more than a conventional "three years and a cloud of dust" research project.

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.

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

CHECRA funding for CMMAP was first allocated in July 2011. It is anticipated that the full \$150,000 will be expended through June 30, 2013. At Colorado State University, CHECRA funds are supporting a percentage of 3 administrative professionals, two research scientists and Dr. Scott Denning. This year CHECRA funding aided in the purchase of additional nodes for the computer cluster, which enhanced CMMAP modeling efforts.

The administrative personnel provide operational support for CMMAP and work diligently toward the Center's sustainability efforts.

The two research scientists who are receiving partial salary support from CHECRA are Ross Heikes and Celal Konor. They work closely together on the development of new mathematical methods to solve the equations of atmospheric motion on the spherical Earth. Their new approach is at the cutting edge of model design, worldwide.

Dr. Denning leads the education and outreach efforts for CMMAP, making presentations to community groups, governmental entities, open public forums and numerous professional organizations. Dr. Denning collaborates on numerous interdisciplinary projects at CSU and educational institutions throughout the United States.

Summary of Benefits to the State of Colorado

- In 2011 the Science and Technology Center (STC) was renewed by NSF through July 2016, in the amount of \$17,991,000 (only STC ever funded in the State of Colorado);
- 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;
- Provided intensive week long training to 45 high school and middle school teachers with the Teaching Weather and Climate Summer Teacher Course;
- Through the Windows to the Universe website had 6,158,872 page views from 4,050,930 visitors;
- Support for 17 CSU graduate students and 12 undergraduate summer interns (3 of these interns are currently considering CSU for graduate school);
- Host CMMAP team meetings in Fort Collins annually bringing over 40 visitors per year to Colorado;
- Hosted and provided content for 2 NSTA webinars focusing on the Earth's climate attended by over 75 science teachers from Colorado and throughout the United States;
- Hosted the Colorado Global Climate Change Conference at Colorado State University attended by over 350 high school students and 20 high school science teachers.

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