

**RESEARCH PROGRAM**  
**Science and Engineering Abstracts**  
**for Grants Awarded in June 2019**

*Columbia University*

*New York, NY*

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*\$1,000,000*

*June 2019*

Since the advent of laser technology, chemical physicists have aspired for bond-specific control of chemical reactions. Applied at ultracold temperatures where quantum effects become important, such control would enable researchers to slice a molecule into desired constituents with an exquisite manipulation of the molecular quantum states. This level of finesse has not yet been achieved because of the experimental and theoretical complexity associated with internal dynamics of even the simplest molecules. Researchers at Columbia and Harvard Universities will pursue a new approach leveraging recent ideas introduced by the PIs and others: separating the goal of species selection from the challenging step of molecular laser cooling by precisely dissociating the desired species from a larger molecule that is amenable to direct cooling. They will develop laser cooling of increasingly complex molecules, and use these to create an unprecedented diversity of ultracold species via bond-specific dissociation, beginning with radicals such as H, OH, CH<sub>3</sub>, and NH<sub>2</sub>. Just as early discoveries in quantum physics changed our daily lives in ways that could not have been predicted, ultracold quantum-mechanical chemistry will lead to valuable applications and fundamental discoveries including searches for new particles that extend the Standard Model as well as high-precision measurements of fundamental constants and their time variations. The techniques pioneered here will revolutionize ultracold chemistry by producing a suite of new molecules and new techniques for steering chemical reactions, and enabling novel experiments that will yield fresh insights into the origins of biomolecular chirality and possibilities of quantum information storage within molecular degrees of freedom.

*Northwestern University  
Evanston, IL  
Andrew Geraci, Vicky Kalogera, Shane Larson  
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The kilometer-scale Laser Interferometer Gravitational-Wave Observatory (LIGO) interferometers have just begun to detect gravitational waves (GWs), firmly establishing the nascent field of GW astronomy. It is paramount to study GW radiation across a wide frequency range, as astronomers have done for visible light and other electromagnetic radiation. While advanced LIGO has achieved remarkable sensitivity at frequencies ranging from 10s of Hz to a few kHz, no established methods can probe the higher frequency part of the spectrum, where undiscovered GW sources may exist, including primordial black holes and other well-motivated dark matter candidates. A team of researchers at Northwestern University aims to develop and test a 1-meter prototype of a novel (GW) detector, based on optically-levitated dielectric particles in an optical cavity. The method could extend the search volume of advanced GW observatories by up to 1000 times in the high frequency (HF) range of 10-300 kHz, using an instrument that is a fraction of their size. To realize the full sensitivity of the detector, the researchers will need to demonstrate trapping and cooling of non-spherical, i.e., disc-like, particles in high vacuum. After initial tests, they will conduct a 1-year observing run using two detectors for frequencies > 10 kHz. The frequency coverage of this instrument complements existing and other proposed GW detectors and promises to enable a new HF-GW map of our universe.

*University of Denver  
Denver, CO  
Mark Siemens, Mark Lusk  
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A team of physicists from the University of Denver and the Colorado School of Mines plan to generate, control, and measure topological fluids made purely of light. Their transformative idea is to treat optical vortices, whirling phase singularities in the light field that have dark centers and quantized angular momentum, as interacting quasiparticles. In this representation, the dynamics are that of an emergent quantum fluid. Vortices and their interactions dominate the properties of turbulent quantum fluids such as superfluid helium and atomic Bose-Einstein Condensates, but it has always been assumed that vortices in light are governed by the optical mode in which they propagate. However, the investigators recently observed emerging quantum fluid behavior and interactions between densely-packed vortices in random light waves (i.e. laser speckle). The very idea that light is a quantum fluid has fascinating foundational implications, which will be probed by exploiting the unprecedented quantum state accessibility of these

topological fluids of light (TFL). Their investigation is a tightly integrated program of computational simulation and experimental measurement to discover and exploit two-body, few-body, and condensed matter dynamics of vortices. In particular, the team seeks to characterize the interaction physics of vortices in a quantum fluid, to diagram the emergent phases of TFL, and to produce vortex structures that exhibit non-abelian anyon behavior needed for topological quantum computing. Topological fluids of light provide exciting new opportunities for exploring and exploiting phenomena that are either difficult to capture or as yet have no counterpart in macroscopic quantum states, a new frontier in topological physics with the potential to enable room-temperature quantum science and computation.

*University of Texas at Austin*

*Austin, TX*

*Sean Roberts, Michael Rose, Joel Eaves*

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*June 2019*

Singlet fission (SF) is a process wherein a molecule in a photoexcited spin-singlet state transfers half of its energy to a neighbor, placing both in an excited spin-triplet state. As SF uniquely excites 2 electrons from a single photon, it has the potential to break barriers that presently limit the efficiency of light harvesting technologies. While the possible utility of SF has been recognized for nearly 40 years, semiconductor devices that leverage SF have not emerged. At the core of this problem is designing effective interfaces that allow spin-triplet excitons (electron-hole pairs) to readily move from an organic SF material to an inorganic semiconductor. This is a challenging problem, as it requires designed interfacial electronic states to serve as an effective interpreting layer, thus allowing localized molecular states to couple with the delocalized states of a bulk semiconductor. The complexity of this process has led some to suggest it is intractable.

This multidisciplinary team of researchers from the University of Texas at Austin and the University of Colorado Boulder is uniquely positioned to tackle the complex problem of triplet transmission across organic|silicon junctions due to their complementary skill-sets. The work plan will simultaneously employ computational methods to identify ideal energy-transmitting organic|inorganic junctions; use advanced synthetic tools to produce these junctions; and experimentally quantify interfacial energy transfer. If successful, this project will not only enable design of new high-efficiency solar cells, displays, and LEDs, but also — quite importantly — create a new platform for testing quantum information transfer and spin entanglement phenomena that will further our fundamental understanding of chemical physics.

*Whitehead Institute for Biomedical Research*

*Cambridge, MA*

*Jing-Ke Weng*

*\$1,000,000*

*June 2019*

In eukaryotes, thousands of metabolic enzymes catalyze diverse chemical reactions that sustain life. Whereas highly efficient natural enzymes evolved over millions of years, humans have made only minimal progress in designing new biocatalysts with desirable functions. An early-career researcher at the Whitehead Institute for Biomedical Research aims to develop a highly efficient and broadly applicable continuous directed evolution system for deriving any metabolic enzyme at will in eukaryotic cells. He plans to harness the interaction between plant viruses and their host plant cells. In this system, the progenitor enzyme-encoding gene to be selected is carried on a crippled version of the viral vector, whereas viral or plant elements necessary for proper viral particle packaging and propagation is placed in the nuclear genome of the host under a regulatable promoter. The system is designed such that serendipitous mutations that steer the progenitor enzyme toward the desirable enzymatic function confer a selective advantage for viral vectors carrying these mutations to propagate more effectively within the host cells. The key innovation is using ligand-regulated transcription factors to link small molecules (products of the selected enzymatic function) to the transcription of the genes that serve as the limiting factors for viral propagation in host cells. Evolving metabolic enzymes at will has been the holy grail in humans' attempts to design synthetic metabolic processes. If successful, this project will have a transformative impact upon multiple fields by enabling the unprecedented capability to create new designer medicines and commodity chemicals.