

**University of California, Berkeley**

Berkeley, CA

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*\$1,000,000*

Dinitrogen gas ( $N_2$ ) accounts for 78% of Earth's atmosphere and is predominantly produced by microbes in soil via denitrification. Directly measuring  $N_2$  fluxes from the terrestrial biosphere is difficult because of high background nitrogen (N) concentration. This missing piece of the N cycle prevents balancing ecosystem N budgets, which greatly limits understanding of other key N cycling processes, including the production and emissions of nitrous oxide ( $N_2O$ ), a potent greenhouse gas, and of nitrogen oxides (NOx) which are precursors to air pollution. The Berkeley team will develop a unique approach to understand and quantify  $N_2$  fluxes and the associated drivers using a combination of isotope biogeochemistry, newly developed printable sensors, and atmospheric and biogeochemical modeling. A continuous  $^{15}N_2O$  pool dilution approach using an isotope cavity ringdown spectrometer coupled to a photoacoustic spectrometer will be used to measure the movement of a  $^{15}N_2O$  label and an  $SF_6$  tracer in real time. NOx fluxes will be measured at the same sites to characterize  $N_2:N_2O:NOx$  partitioning. Novel printed 3D sensors will be used to measure drivers of N fluxes at high temporal and spatial resolution. These measurements will form the foundation of new ideas and computational models that allow description of the N-cycle on time scales from seconds to centuries as needed to understand the controls over ecosystem processes and the history of Earth's atmosphere.

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**Emory University**

Atlanta, GA

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This project will explore a grossly undeveloped subject: how microbes survive, grow, and interact in the air. The research is motivated by overwhelming evidence that airborne microbes critically impact everyday life, e.g., rainfall, disease spread, land fertilization, and food production. Furthermore, detailed studies of airborne microbiota are essential for understanding Earth's ecosystems. However, current studies mostly dwell on soil/marine microbiota. The challenge of studying airborne microbes is obvious: how can microbes be cultured in the air? An interdisciplinary team, with researchers from Emory University and the University of Oregon, recently developed a prototype acoustic levitation system that opens the door for air-culturing microbes in a well-controlled laboratory condition for the first time. The project has three goals: 1) to develop and optimize this levitation system to be amenable to biological experiments; 2) to collect airborne microbes and characterize

their environment using ultra-light balloons and develop a repository of airborne microbes; and 3) to conduct the first-ever laboratory experiments of airborne microbiology. The expected outcome is a detailed understanding of the physiology, metabolism, ecology, and evolution of airborne microbes. The innovative and rich resources developed throughout this project will be open source, which will strengthen research infrastructure in this underdeveloped field. Additionally, this research will have a transformative impact on our fundamental understanding of biological processes taking place in the atmosphere and more broadly, Earth's ecosystems. Ultimately, this improved understanding can be leveraged to predict global effects of airborne microbes, ranging from meteorological processes to public health and agriculture.

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**Rice University***Houston, TX**Hanyu Zhu, Kaden Hazzard, Junichiro Kono**\$1,200,000*

Conventionally, quantum physics governing elementary particles will reduce to classical physics in macroscopic objects containing billions of particles. An exciting scientific and engineering frontier is to create and utilize effects unique to the quantum regime, such as entanglement, at a macroscopic scale. In addition to scientific interest, these effects are the basis for promising technologies that outperform those relying on only classical ones. Theory predicts that a phenomenon in macroscopic materials called ultrastrong coupling can lead to intrinsic, perfect quantum squeezing, which ensures entanglement, without the need of active control. The team at Rice University recently discovered that the coupling between spins on rare-earth atoms and the spin waves (magnons) on iron atoms is ultrastrong and tunable in bulk crystals of rare-earth orthoferrites ( $R\text{FeO}_3$ , R: rare-earth element). Their calculations suggest that it is possible to control the materials with external fields and spontaneously create a squeezed spin-magnon field in the ground state. The researchers plan to experimentally create and probe squeezing at an unprecedentedly large scale by directly measuring and altering the quantum fluctuations of spins and magnons, which can then reveal their entanglement. Ideally, tuning the system to a critical point will eliminate quantum noise in a particular physical variable of the spin-magnon ground state. (The state still preserves the Heisenberg uncertainty principle by developing diverging fluctuations in its conjugate variable.) The team will systematically search for the material compositions, external control parameters, and experimental conditions that maximize such ground-state squeezing. In parallel, they will develop optomagnonics protocols to perform precise quantum weak measurement of the spin-magnon fluctuations. The team will also build comprehensive models that incorporate the experimentally observed coherence properties to analyze the depth of squeezing and entanglement, and thus ultimately elucidate the quantum to classical crossover in solid-state systems. Owing to its fundamental stability, such intrinsic and macroscopic squeezing, if realized in materials, has the potential to revolutionize quantum sensing and continuous-variable quantum information technologies.

**Rutgers University***New Brunswick, NJ**Sang-Wook Cheong, Valery Kiryukhin, Sang-Hyuk Lee, Andrei Sirenko**\$1,100,000*

Today's digital technology uses binary logic with only two states: on or off. Imagine how society would be transformed if we had devices with thousands of logical states that are coupled together! Dramatic improvements in power consumption and density of computing elements can be achieved by multinary technology utilizing topologically protected ensembles of electron spins. While coupling and control of topological spin ensembles are inaccessible to standard probes, such as conventional light, this team of researchers from Rutgers University and the New Jersey Institute of Technology propose a new paradigm: using topological vortex light with orbital angular momentum (OAM). They hypothesize that only a probe with the topology, energy, and length scale matching the topological quantum spin ensembles can couple effectively to those spin ensembles. Vortex beams meet these requirements, and the team's initial discoveries in the THz energy range support this hypothesis. The researcher's objectives include creating, reading, and manipulating previously inaccessible quantum spin states with vortex beams using a wide range of OAM (up to a thousand). Examples include topologically-protected chiral spin textures, vortices, skyrmions, hopfions, and quantum Hall states with multi-valued topological indices. Specifically, they will attempt to: understand the mechanism of and optimize the coupling between THz, visible, and x-ray vortex beams and topological spin states; explore the dynamics of topological transitions in quantum spin states by vortex beams; and, attempt preliminary multinary device implementation of their scientific discoveries. This work is expected to have tremendous impact on its scientific field and society, opening new frontiers in quantum magnetism, enabling innovative multinary electronics, and influencing artificial intelligence.

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**University of Utah***Salt Lake City, UT**Michael Gruenwald, Ryan Looper, Rodrigo Noriega**\$1,000,000*

Predicting the crystal structures of molecules is an extraordinarily difficult problem that cannot be solved using thermodynamics alone. However, calculating crystallization kinetics is notoriously challenging. This work seeks to establish a new paradigm in crystal structure prediction that accounts for differences in the crystallization rates of molecular systems by focusing on the oligomeric species that they form in solution. The strategy tightly integrates computer simulations, analysis of crystal structures, experimental crystallization screenings, and spectroscopy. The overarching goal is to demonstrate that solution oligomers play an important role in the crystallization of typical organic molecules and that their inclusion in crystallization models can markedly improve crystal structure prediction based solely on energy landscapes. The main hypothesis is that decisive differences in polymorph formation kinetics can be estimated at moderate cost by

analyzing correlations between structural motifs within predicted low-energy structures and molecular clusters in solution. This project will develop kinetic models for crystal structure prediction that allow ranking of predicted low-energy crystal structures according to relative crystallization rates. This research should pave the way for new, more accurate structure prediction methods able to select experimentally viable polymorphs from potentially long lists of predicted low-energy structures, predict changes in crystallization behavior depending on solution conditions, and provide useful information even in the absence of accurate crystal energies. When applied in industrial and pharmaceutical settings, these methods will likely reduce the need of time- and resource intensive solid-form screenings, reduce drug development times, and facilitate the discovery of new organic materials.