2nd Annual CMQT Symposium

CMQT
CENTER FOR MOLECULAR QUANTUM TRANSDUCTION

Northwestern University
April 21-22, 2022

Northwestern | INSTITUTE FOR SUSTAINABILITY AND ENERGY


Northwestern

Welcome

Dear Participants,

The mission of the Center for Molecular Quantum Transduction (CMQT) is to develop the fundamental scientific understanding needed to carry out quantum-to-quantum transduction through a bottom up synthetic approach that imparts atomistic precision to quantum systems. Quantum transduction is the coherent exchange of information between quantum systems, such as photons and electron spins, and is essential for establishing coherent communications between quantum processing nodes and sensors.

On behalf of the Institute for Sustainability and Energy at Northwestern (ISEN) and CMQT, we are delighted to welcome you to the 2nd Annual CMQT Symposium.

We have an impressive group of speakers for this year's Symposium, who are amongst the leaders in quantum information science and technology. These scientific leaders will present state-of-the-art approaches to novel quantum materials, measurements, and theory relevant to quantum transduction.

Please join us for the entire day, or just for one talk—whatever your schedule may permit. We hope that you will arrive with an open mind, ask questions while you are here, and leave feeling engaged and informed.

Sincerely,

Michael R. Wasielewski
Clare Hamilton Hall Professor of Chemistry, Northwestern University
Director, CMQT
Executive Director, ISEN

Agenda

Thursday, April 21

Pancoe Auditorium, 2200 Campus Dr., Evanston, IL 60201 // Zoom

5:00pm	**Keynote Address with Prineha Narang** **Harvard University** "Ab Initio Approaches to Molecular Quantum Matter and Quantum Information Science"

Friday, April 22

Norris University Center, 1999 Campus Dr., Evanston, IL 60208 // Zoom

9:00am	**Welcome (Location: 100 McCormick Auditorium)**
9:15am	**Peter Maurer, University of Chicago** "Quantum Sensing: Probing Biological Systems in a New Light"
10:00am	**Elizabeth Goldschmidt, University of Illinois Urbana-Champaign** "Emerging Rare-Earth Materials for Optical Quantum Information Science"
10:45am	Break
11:15am	**Theodore Goodson, University of Michigan** "Nonlinear and Quantum Optical Properties of Novel Functional Organic Materials"
12:00pm	Lunch - Options in the basement of Norris University Center PI's & Symposium Speakers: 102 Evans Room
1:00pm	**Kwabena Bediako, University of California Berkeley** "New Twists on Chemistry and Physics in Atomically Layered Materials"
1:45pm	**Jeffrey Thompson, Princeton University** "Quantum Technologies with Rare Earth Ions"
2:30pm	Break
3:00pm	**Sophia Economou, Virginia Polytechnic Institute and State University** "Simulating Many-Body Systems with Near-Term Quantum Computers"
3:45pm	**Poster Session (Location: 101 Wildcat Room)**

Keynote Speaker - Prineha Narang

Assistant Professor of Computational Materials Science – Harvard University

Dr. Prineha Narang leads an interdisciplinary group working on topics at the vibrant intersection of theoretical and computational quantum materials science, condensed matter physics, and quantum photonics. She received an M.S. and Ph.D. in Applied Physics from the California Institute of Technology (Caltech) supported by a Resnick Fellowship and an NSF Graduate Fellowship. Dr. Narang's work has been recognized by many awards and special designations, including the Mildred Dresselhaus Prize, Bessel Research Award from the Alexander von Humboldt Foundation, a Max Planck Sabbatical Award from the Max Planck Society, and the IUPAP Young Scientist Prize in Computational Physics, an NSF CAREER Award and a DOE INCITE Award, being named a Moore Inventor Fellow by the Gordon and Betty Moore Foundation for pioneering innovations in quantum science, CIFAR Azrieli Global Scholar by the Canadian Institute for Advanced Research, a Top Innovator by MIT Tech Review (MIT TR35), and a leading young scientist by the World Economic Forum. Dr. Narang holds leadership roles in the DOE EFRC 'Photonics at Thermodynamic Limits' and DOE NQI Quantum Science Center, among others. She is also the founder and Chief Technology Officer of Aliro, a VC-backed US quantum network company.

Abstract: This talk presents a pedagogical introduction to theoretical and computational approaches to describe excited-states in quantum matter, and predicting emergent states created by external drives. Understanding the role of such light-matter interactions in the regime of correlated electronic systems is of paramount importance to fields of study across condensed matter physics, quantum optics, and quantum chemistry. The simultaneous contribution of processes that occur on many time and length-scales have remained elusive for state-of-the-art calculations and model Hamiltonian approaches alike, necessitating the development of new methods in theoretical and computational quantum chemistry. I will discuss our work at the intersection of ab initio cavity quantum-electrodynamics

and electronic structure methods to treat electrons, photons and phonons on the same quantized footing, accessing new observables in strong light-matter coupling. Current approximations in the field almost exclusively focus on electronic excitations, neglecting electron-photon effects, for example, thereby limiting the applicability of conventional methods in the study of quantum chemical and polaritonic systems, which requires understanding the coupled dynamics of electronic spins, nuclei, phonons and photons. With our approach we can access correlated electron-photon and photon-phonon dynamics. I will demonstrate this approach in two contexts relevant to control of molecular quantum matter and molecular quantum transduction.

Kwabena Bediako
Assistant Professor of Chemistry - University of California Berkeley; Lawrence Berkeley National Laboratory

Kwabena was born in Ghana, West Africa. He moved to the US in 2004 for his undergraduate studies in Chemistry at Calvin College, MI, graduating with honors in 2008. After a year working at UOP Honeywell in IL where he researched new catalysts for the petrochemical and gas processing industries, he traveled from the Midwest to the East Coast to begin his graduate studies in Inorganic Chemistry with Prof. Daniel Nocera at MIT (and later Harvard University). His graduate research focused on structural and mechanistic studies of water splitting electrocatalysis at cobalt and nickel compounds. After receiving his Ph.D. in 2015 from Harvard University, Kwabena began postdoctoral work in Prof. Philip Kim's group in the Department of Physics at Harvard, where he studied ion intercalation and quantum transport in 2D van der Waals heterostructures. In July 2018, Kwabena joined the faculty of the UC Berkeley Department of Chemistry. Awards received include: AFOSR and ONR Young Investigator awards, DOE Early Career Award, and Gordon and Betty Moore Materials Synthesis Fellow.

Abstract: Atomically thin or two-dimensional (2D) materials can be assembled into bespoke heterostructures to produce

some extraordinary physical phenomena. Likewise, these highly tunable materials are useful platforms for exploring fundamental questions of interfacial chemical/electrochemical reactivity. One exciting and relatively recent example is the formation of moiré superlattices from azimuthally misoriented (twisted) layers. These moiré superlattices result in flat bands that lead to an array of correlated electronic phases. However, in these systems, complex strain relaxation can also strongly influence the fragile electronic states of the material. Precise characterization of these materials and their properties is therefore critical to the understanding of the behavior of these novel moiré materials (and 2D heterostructures in general). In this talk, I will discuss how spontaneous mechanical deformations (atomic reconstruction) and resultant intralayer strain fields at moiré superlattices of twisted bilayer graphene have been quantitatively imaged using 4D-STEM Bragg interferometry. I will also discuss the impact of these mechanical deformations to the electronic band structure of these moiré superlattices and the correlated electronic phases they host. The talk will then explore how various degrees of freedom that are unique to 2D materials may be used to tailor interfacial chemistry at well-defined mesoscopic electrodes and the outlook for new paradigms of functional materials for energy conversion and low-power electronic devices.

Sophia Economou

Professor of Physics - Virginia Polytechnic Institute and State University

Sophia Economou is a Professor of Physics and the Hassinger Senior Fellow of Physics at Virginia Tech. She is also the founding director of the Virginia Tech Center for Quantum Information Science and Engineering. Her research focuses on theoretical aspects of quantum information science, including quantum computing, quantum communications, and quantum simulation algorithms.

Abstract: The simulation of strongly correlated systems is one of the most exciting potential applications of quantum computers. There is hope that variational algorithms could enable the simulation

of classically intractable problems on near-term devices, but this requires significant advances, both in the hardware and in the algorithms. I will discuss recent efforts to lower these resource demands using adaptive algorithms, symmetry considerations, and control-based methods.

Elizabeth Goldschmidt
Assistant Professor of Physics - University of Illinois Urbana-Champaign

Elizabeth Goldschmidt is an assistant professor of physics at the University of Illinois Urbana-Champaign. Her research interests include hybrid systems for quantum networking, solid-state optical emitter platforms for quantum memory and other applications in quantum information science, and single photon technologies. Before joining the faculty at UIUC, Elizabeth was a staff physicist at the US Army Research Lab and a postdoctoral fellow at the National Institute of Standards and Technology. She received her PhD in physics from the University of Maryland in 2014 and her AB in physics from Harvard University in 2006.

Abstract: Optically active and highly coherent emitters in solids are a promising platform for a wide variety of quantum information applications, particularly quantum memory and other quantum networking tasks. Rare-earth atoms, in addition to having record long coherence times, have the added benefit that they can be hosted in a wide range of solid-state materials. We can thus target particular materials (and choose particular rare-earth species and isotopes) that enable certain application-specific functionalities. I will discuss several ongoing projects with rare-earth atoms in different host materials and configurations. This includes investigations of inhomogeneous broadening in rare-earth ensembles, which is highly host-dependent and plays an important role in the quantum memory protocols that can be implemented in any given system. I will present results on our efforts to identify and grow new materials with rare-earth atoms at stoichiometric concentrations in order to reduce the disorder-induced inhomogeneous broadening. I will also discuss our work

investigating photonic integration of rare-earth doped samples that aims to increase the light-atom interaction for practical quantum devices. I will show results from our work with rare-earth atom dopants in thin-film lithium niobate, which admits standard nanofabrication techniques, and show the suitability of this platform for quantum applications.

Theodore Goodson III

Richard Barry Bernstein Collegiate Professor of Chemistry and Macromolecular Science and Engineering - University OF Michigan

The Goodson research group utilizes a number of spectroscopic techniques towards investigating the optical properties and applications of novel organic macromolecular materials. A major emphasis is placed on the new properties observed in organic macromolecules with branching repeat structures as well as organic macromolecules encapsulated with small metal particles. These materials have been suggested to be candidates for variety of applications involving light emitting devices, artificial light harvesting, strong optical limiters, enhanced nonlinear optical effects, quantum optical effects and as sensors in certain organic and biological devices.

Abstract: Organic conjugated molecules for optical and electronic applications have received great attention due to their versatility and relatively low manufacturing costs. While there has been great improvement of light conversion efficiency in certain photovoltaic materials, there still remain questions concerning the structural and inhomogeneity of the electron and energy transport processes. In this regard, understanding the fast processes (fs) at a local level (nm) in these systems is crucial in the design criteria for better performance in optical and electronic applications. In this presentation, the results of photo-physical dynamics of organic and inorganic light harvesting materials will be described. These materials have been analyzed using time-resolved absorption and fluorescence spectroscopy and microscopy as well as a nonlinear and quantum optical spectroscopy. Ultra-fast interferometric microscopic measurements were carried out to investigate the

role of coherent energy transport in these organic photovoltaic materials. The use of these methods provide insights in to the dynamics and degree of heterogeneity in novel organic materials for optical and electronic applications.

Peter Maurer

Assistant Professor of Molecular Engineering - University of Chicago

Peter Maurer's research interests lay at the interface of quantum engineering and biophysics. His lab at the University of Chicago uses quantum technology to develop novel sensing modalities that allow us to probe physical properties of biological systems that are not accessible by conventional technologies. Specific examples of such quantum technology includes a nanoscale magnetic field sensor that enables probing nuclear magnetic resonance (NMR) spectroscopy of picoliter volumes. Recent results from the Maurer lab have shown that these coherent quantum sensors can be interfaced with intact biomolecules (*M. Xie, et al., PNAS (2022)*). Among others, the resulting advances open the door to performing NMR spectroscopy on protein samples at physiological concentrations. Currently the Maurer lab is working with SomaLogic, a startup company, to utilize this technology as a platform for high-throughput proteomics. Prior to joining the faculty at the University of Chicago, Peter received his postdoctoral training working with Steven Chu at Stanford University and his PhD training working with Mikhail Lukin at Harvard University.

Abstract: Quantum optics has had a profound impact on precision measurements, and recently enabled probing various physical quantities, such as magnetic fields and temperature, with nanoscale spatial resolution. In my talk, I will discuss the development and application of novel quantum metrological techniques that enable the study of biological systems in a new regime. I will start with a general introduction to quantum sensing and its applications to nanoscale nuclear magnetic resonance (NMR) spectroscopy. In this context, I will discuss how we can utilize tools from single-molecule biophysics to interface a coherent quantum sensor with individual

intact biomolecules, and how this could eventually pave the way towards a new generation of biophysical and diagnostic devices.
In a second part, I will discuss a theoretical proposal that utilizes variational techniques to drive a dipolar interacting spin ensemble into a metrological relevant state with Heisenberg limited sensitivity.

Jeff Thompson

Associate Professor of Electrical and Computer Engineering - Princeton University

My research explores methods to gain control over individual atoms for computing, communications and sensing technology. When isolated, atoms display manifestly quantum mechanical behavior, routinely doing things like being in two places at the same time or getting entangled with their neighbors. In macroscopic clumps like computer chips, these effects are washed out. However, there is strong motivation to try to build computers and communications devices in such a way that the quantum properties of individual atoms can be retained because devices operating according to quantum laws can offer dramatic advantages in terms of power and security. We focus on two types of isolated atoms: atoms levitated in vacuum and impurities in otherwise perfect crystals. In both cases, we use nano-fabricated optical structures as a microscope that allows us to resolve these atoms, and to prepare and measure their quantum states using photons. Additionally, these photons can be used to create interactions and entanglement between atoms.

In one research direction, we are using nanophotonic circuits to spatially isolate and address individual or small clusters of rare earth ion dopants in crystalline hosts for use as single photon sources and quantum memories. These are crucial ingredients for quantum repeater systems for quantum communications networks. In connection with this research, we are also working on basic engineering for other components of a complete quantum repeater architecture, such as high-Q photonic crystal cavities, fiber-chip interconnects, wavelength converters and ultra-low-noise single photon detectors.

In a second research direction, we are developing techniques to laser-cool and trap large arrays of atoms levitated in vacuum. The potential to create very uniform and homogeneous arrays with long-range photon-mediated interactions creates many possibilities for studies of quantum many-body physics and new quantum computing architectures.

Abstract: Atomic defects in solid-state crystals are widely explored as single-photon sources and quantum memories for large-scale quantum communications networks based on quantum repeaters. Rare earth ions, in particular Er3+, have attracted recent attention because of the demonstration of extremely large Purcell enhancement in nanophotonic cavities, which overcomes the slow intrinsic photon emission rate. Using this approach, we have demonstrated the first atomic source of single photons in the telecom band, and high-fidelity single-shot readout of the Er^{3+} electron spin using cavity-induced cycling transitions. Furthermore, we have realized optical manipulation and single-shot readout of multiple atoms with spacings far below the diffraction limit of light, using a novel frequency-domain super-resolution technique. I will conclude by discussing some recent work on coherent control of nearby nuclear spins, as well as a systematic investigation of new host materials with the potential to realize longer spin and optical coherence times.

Michael R. Wasielewski

Director of CMQT; Executive Director of ISEN; Clare Hamilton Hall Professor of Chemistry - Northwestern University

Michael R. Wasielewski is currently the Clare Hamilton Hall Professor of Chemistry at Northwestern University, Executive Director of the Institute for Sustainability and Energy at Northwestern, and Director of the Center for Molecular Quantum Transduction, a US-DOE Energy Frontier Research Center. He received his B.S., M.S., and Ph.D. degrees from the University of Chicago and was a postdoctoral fellow at Columbia University. His research has resulted in over 750 publications and focuses on light-driven processes in molecules and materials, artificial photosynthesis, molecular electronics, quantum information science, ultrafast optical spectroscopy, and time-resolved electron paramagnetic resonance spectroscopy. His honors and awards include membership in the National Academy of Sciences and the American Academy of Arts and Sciences; the Josef Michl American Chemical Society Award in Photochemistry; the Porter Medal for Photochemistry; the James Flack Norris Award in Physical Organic Chemistry of the American Chemical Society; the Royal Society of Chemistry Physical Organic Chemistry Award; the Royal Society of Chemistry Environment Prize; the Arthur C. Cope Scholar Award of the American Chemical Society; the Bruker Prize in EPR Spectroscopy; the International EPR Society Silver Medal in Chemistry; the Chemical Pioneer Award of the American Institute of Chemists; and the Humboldt Research Award.

CMQT Overview

CMQT's Mission

The mission of the Center for Molecular Quantum Transduction (CMQT) is to develop the fundamental scientific understanding needed to carry out quantum-to-quantum transduction through a bottom-up synthetic approach, which imparts atomistic precision to quantum systems.

CMQT's Vision

Achieving molecular quantum-to-quantum transduction is necessarily an interdisciplinary effort, requiring necessary expertise in the design and synthesis of molecular and solid-state materials, the capacity to measure coherent quantum states at the single quantum level, and the ability to seamlessly incorporate theory and modeling of materials and measurement schemes with the experimental constraints of real systems.

CMQT's team of chemists, physicists, and materials scientists has been assembled with exactly this challenge in mind. Each team member brings a suite of experimental and theoretical tools to bear that have been extensively validated by CMQT's preliminary research and a history of successful collaborations with one another.

To achieve its mission, CMQT researchers study the underlying interactions among quantum spins, excitons, and vibrational excitations of molecules and molecular materials that are relevant to molecular quantum-to-quantum transduction. CMQT comprises an interdisciplinary team with the individual expertise and collective breadth to create knowledge in this emerging area. Understanding and achieving quantum-to-quantum transduction, an essential element of quantum information science, is a key priority for the U.S. Department of Energy.

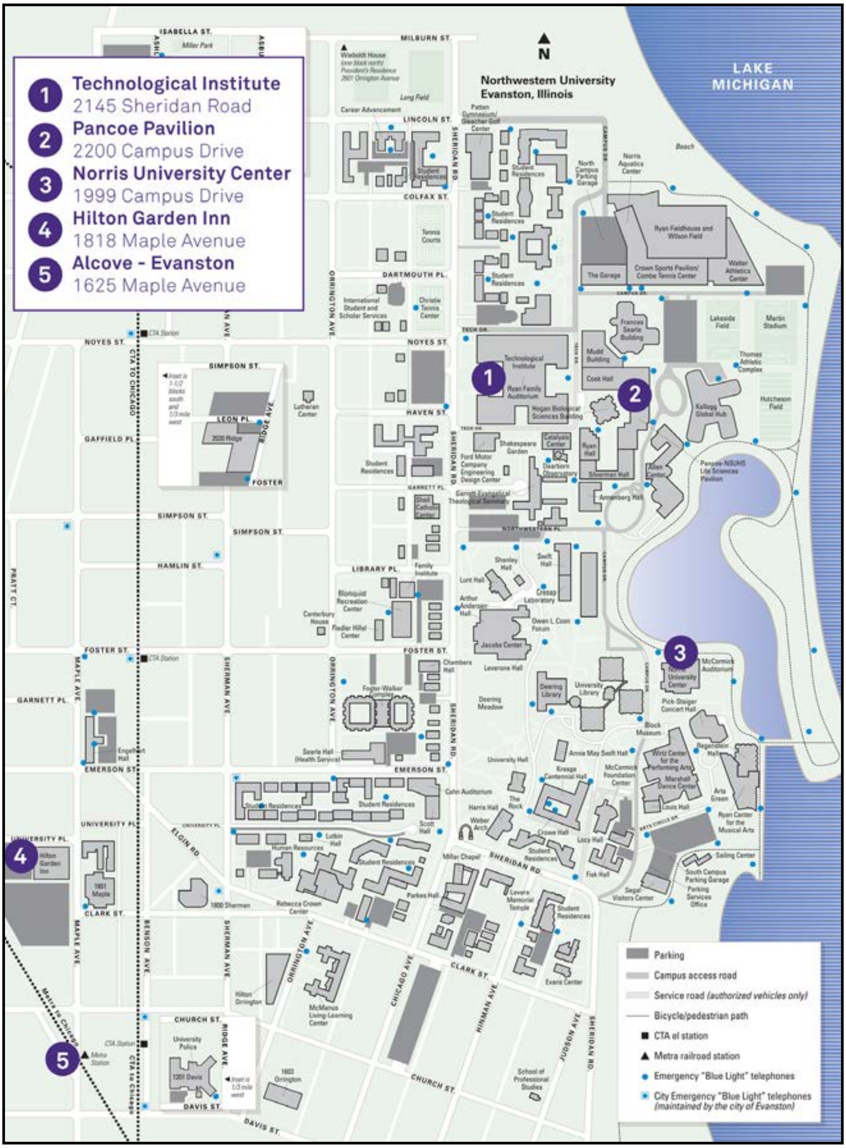
CMQT Research Strategy

The CMQT research team's approach includes both ensemble-level studies to rapidly understand interactions and the development of single-molecule methods to interface molecular Quantum Information Science (QIS) with other QIS platforms. CMQT is also leveraging cutting-edge physical measurement techniques with high spatial, temporal, and spectral resolution to understand how to transition quantum-to-quantum transduction from the ensemble to the single molecule level.

CMQT comprises three cross-cutting Research Thrusts with closely integrated approaches and team synergies that progressively exploit the flexibility and tunability of molecular architectures to address quantum-to-quantum transduction at increasing length scales. Individually, the Thrusts each pose and answer fundamental questions relevant to quantum transduction in different regimes, ranging from local to long-distance. Taken together, the Thrusts develop a transformative integrated framework for how molecules can facilitate quantum transduction at all the scales relevant for quantum information science.

Thank you for joining us for the 2nd Annual CMQT Symposium

Event Map



1 Technological Institute
2145 Sheridan Road
2 Pancoe Pavilion
2200 Campus Drive
3 Norris University Center
1999 Campus Drive
4 Hilton Garden Inn
1818 Maple Avenue
5 Alcove - Evanston
1625 Maple Avenue
N
Northwestern University
Evanston, Illinois
LAKE MICHIGAN
Parking
Campus access road
Service road (authorized vehicles only)
Bicycle/pedestrian path
CTA el station
Metra railroad station
Emergency "Blue Light" telephones
City Emergency "Blue Light" telephones (maintained by the city of Evanston)


University

Northwestern | INSTITUTE FOR SUSTAINABILITY AND ENERGY

CMQT
CENTER FOR MOLECULAR QUANTUM TRANSDUCTION

The Center for Molecular Quantum Transduction (CMQT), a strategic research center at the Institute for Sustainability and Energy at Northwestern (ISEN), develops the fundamental scientific understanding needed to carry out quantum-to-quantum transduction through a bottom-up synthetic approach, which imparts atomistic precision to quantum systems.

ISEN's mission is to advance global sustainability and energy solutions through transformational research, interdisciplinary education, and public engagement.

Technological Institute
2145 Sheridan Rd, L410
Evanston, Illinois 60208

isen.northwestern.edu/cmqt
@ISENatNU