



Graduate Research Cooperative

Profiles of Argonne scientists who are approved to work with University of Chicago graduate students through the GRC initiative:



Khalil Amine, Ph.D.

- Head of the Technology Development group in the Electrochemical Energy Storage Department within Argonne National Laboratory's Chemical Sciences and Engineering Division

Website: [Argonne profile](#)

Research interests: New materials for next-generation batteries.



Edward F. Barry, Ph.D.

- Applications Scientist / Physicist, Applied Materials Division (AMD), Argonne National Laboratory
- Research Integration Officer for the Advanced Materials for Energy-Water Systems EFRC
- Director of Communications, DOE Energy I-Corps Alumni Association

Website: [Argonne profile](#)

Research interests: Soft matter, materials science, energy storage, water.
[Learn more.](#)



Anand Bhattacharya, Ph.D.

- Physicist at Argonne National Laboratory

Website: [Argonne profile](#)

Research interests: Novel electronic and magnetic properties that emerge in epitaxial thin films and heterostructures of various crystalline materials.



Wei Chen, Ph.D.

- Chemist at Materials Science Division (MSD), Center for Molecular Engineering (CME), and Advanced Materials for Energy-Water Systems (AMEWS) Center, Argonne National Laboratory

Website: [ORCID profile](#)

Research interests: Precise Polymer Synthesis, Soft Matter Interfaces, X-ray and Neutron Scattering. [Learn more.](#)



Justin G. Connell, Ph.D.

- Manager of the Electrochemical Discovery Laboratory and Materials Scientist in the Joint Center for Energy Storage Research (JCESR) Energy Innovation Hub at Argonne National Laboratory

Website: [Laboratory homepage](#)

Research interests: Interfacial Electrochemistry and Ultrahigh Vacuum Materials Synthesis and Characterization. [Learn more.](#)



Seth B. Darling, Ph.D.

- Director of the Center for Molecular Engineering
- Director of the Advanced Materials for Energy-Water Systems EFRC
- Senior Scientist in the Chemical Sciences and Engineering (CSE) Division at Argonne National Laboratory and Senior Scientist at the Pritzker School of Molecular Engineering at the University of Chicago

Website: [Google Scholars page](#)

Research interests: New materials for water treatment. [Learn more.](#)



Jeffrey Elam, Ph.D.

- Group Leader, Argonne National Laboratory's Functional Coatings Group in the Applied Materials division

Website: [Argonne profile](#)

Research interests: Coating technologies for a diverse range of applications, including energy storage, photodetectors, and water purification.



Marco Govoni, Ph.D.

- Assistant Scientist in the Materials Science Division at Argonne National Laboratory and Pritzker School of Molecular Engineering

Website: [Argonne profile](#)

Research interests: Predictive modeling techniques based on first principles numerical simulations to help design advanced materials for renewable energy, water, and quantum information technologies



Joseph Heremans, Ph.D.

- Staff scientist at Argonne National Laboratory

Website: [Argonne profile](#)

Research interests: Engineering spin systems in diamond, silicon carbide, and other wide bandgap semiconductors for quantum information, nanoscale sensing, and quantum communication applications



Stephan O. Hruszkewycz, Ph.D.

- Group Leader of the Synchrotron Studies of Materials Group
- Physicist in the Materials Science Division at Argonne National Laboratory

Website: [Argonne profile](#)

Research interests: Microscopy of quantum materials with coherent x-rays, numerical methods for inverse diffraction problems. [Learn more.](#)



Di-Jia Liu, PhD.

- Senior Chemist and Principal Investigator in the Catalysis and Energy Conversion group at Argonne National Laboratory
- Senior Fellow at Pritzker School of Molecular Engineering

Website: [Argonne profile](#)

Research interests: Nanomaterials for fuel cells, electrocatalysis for water splitting, CO₂-to-chemical/fuel conversion, hydrogen/methane storage, lithium-air battery, energy-water research.



Xuedan Ma, Ph.D.

- Assistant Scientist, Nanoscience, at Argonne National Laboratory

Website: [Argonne profile](#)

Research interests: Quantum optics of semiconductor nanomaterials, excitonic and electronic properties of optically active materials, plasmonic and dielectric metamaterials; nanophotonics and nano-optics, high-resolution single molecule/particle optical spectroscopy and imaging.



Alex B. F. Martinson, Ph.D.

- Chemist in the Materials Science Division (MSD) at Argonne National Laboratory
- Principal investigator & thrust co-leader of Advanced Materials for Energy-Water Systems EFRC and Light Energy Activated Redox Processes EFRC

Website: [Google Scholar page](#)

Research interests: Surface chemistries and optoelectronic processes that occur at the interface between materials. [Learn more.](#)



Orlando Quaranta, Ph.D.

- Physicist of the Detectors Group at the Advanced Photon Source at Argonne National Laboratory
- UChicago-CASE Scientist at the Pritzker School of Molecular Engineering at the University of Chicago.

Website: [Google Scholar page](#)

Research interests: Superconducting micro- and nano-devices. [Learn more.](#)



Subramanian Sankaranarayanan, Ph.D.

- Group Leader, Theory and Modeling Group, at Argonne National Laboratory

Website: [Argonne profile](#)

Research interests: Machine learning to bridge the electronic, atomistic and mesoscopic scales, integrating atomistic (and continuum) simulations with ultrafast X-ray imaging, inverse design for materials discovery and machine learning to predict metastable phase diagrams.



Martin Suchara, Ph.D.

- Scientist in the Mathematics and Computer Science division at Argonne National Laboratory and at the Pritzker School of Molecular Engineering at the University of Chicago

Website: [Google Scholar page](#)

Research interests: Quantum computing and networking. [Learn more.](#)

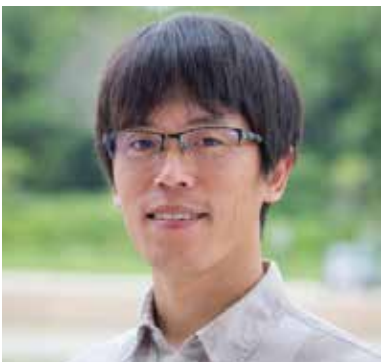


Jie Xu, Ph.D.

- Assistant Scientist in Nanoscience and Technology (NST) Division at Argonne National Laboratory

Website: [Google Scholar page](#)

Research interests: Understanding and controlling polymer packing under non-equilibrium state with desired and new properties. [Learn more.](#)



Xufeng Zhang, Ph.D.

- Assistant Scientist at Argonne National Laboratory

Website: [Argonne profile](#)

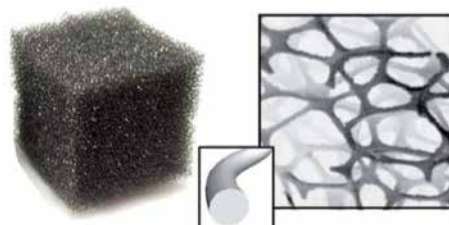
Research interests: Experimental study of hybrid quantum systems involving magnon spintronics, integrated photonics, and nanomechanics, aiming at developing high-fidelity quantum transducers for distributed quantum networks.



Edward F. Barry, Ph.D.

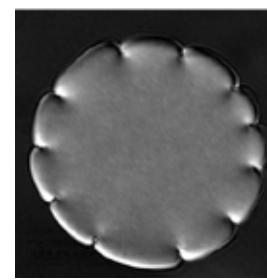
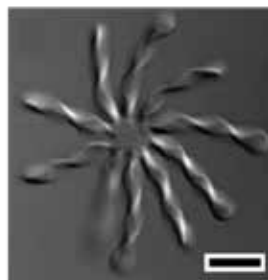
Materials Design for Separations and the Energy-Water Nexus

This research is based on the synthesis of hybrid inorganic/organic materials for fundamental studies in separations and applications in water and energy storage. Building off the success of the OleoSponge - a reusable oil adsorbent based on polymeric foam, we investigate general methods of atomic layer deposition and subsequent surface chemistry functionalization routines as a means by which to engineer highly specific and robust materials. The methods employed allow us to generate material platforms with direct control over material properties from sub-nanometer to centimeter length scales in a variety of different form factors (e.g. solid state nanopores, membranes, foams). We explore a range of functionalization motifs, including chemistries tailored for ionic sorption in aqueous solution (e.g. capacitive deionization and desalination), as well complex chemistries for advanced energy storage devices. At the heart of such studies is novel material design strategies for model and applied systems, that can better our fundamental understanding of interfacial phenomena in confined geometries, and can generate materials for a wide range of practical applications, including sensors, sorbents, and ion selective membranes.



Biomolecular Soft Matter Physics

This research is focused on the discovery, design and synthesis of functional materials and complex structures based on principles and concepts of biology. As general themes, we seek to mimic Nature's ability in assembling micro- and meso-scopic structures with remarkable specificity and complexity, and use these features to engineer materials that display complex yet well-coordinated collective behavior. Specific examples include new classes of hypercomplex fluids based on filamentous viruses, bacterial flagella, and other biological building blocks that can respond to chemical, optical, electronic, and/or mechanical signals, with applications in energy relevant materials, and multi-component classes of reconfigurable materials that are resilient, can transfer energy, and control transport.



Technology Maturation and Commercialization



There are a number of exciting opportunities at the University of Chicago and Argonne National Laboratory for technology development and commercialization. Our group actively engages in a number of these activities, with the overall goal of training scientists to become chief technical and executive officers of their own startups using technologies developed in the lab. Such activities include placing a strong emphasis on intellectual property and patenting, strong interactions and collaboration with industry, as well as participation in the UChicago Polsky Center for Innovation and the DOE Energy I-Corps program.



Wei Chen, Ph.D.

Structures, Dynamics and Transport at Soft Interfaces in Ionic Environments

- Determine ion distribution in polyelectrolyte and polyzwitterionic brushes and their counterions at solid-liquid interfaces through resonant anomalous x-ray scattering and contrast variation neutron scattering
- Understand complex intermolecular interactions at interfaces and formation of interfacial complexes that affect the dynamics of particles and self-assembled block copolymers
- Design and implement the in situ shearing X-ray measurement system, operated at the APS to investigate the structures and dynamics of end-tethered polymers at the solid-liquid interface and correlate particle-scale phenomena to the rheology of multiphase larger-scale systems

Modulation of Interfacial Charge Transport for Ultralow Power Electronics

- Sub-volt reversible manipulation of phase transitions of functional metal oxides through poly(ionic liquid)-based redox gating
- Avoid unwanted electrochemistry at heterointerfaces
- Enhanced tunability (induced carrier density $\sim 10^{14} - 10^{15}$)
- Improved reversibility
- Achieve novel functionalities



Justin G. Connell, Ph.D.

Interfacial Electrochemistry of Anodes and Cathodes for Beyond Li-Ion Batteries

Energy storage systems that move beyond current Li-ion technologies are critical to enabling the widespread electrification of transportation and the integration of intermittent renewable energy sources into the grid. Batteries that make use of multivalent ions such as magnesium and calcium serve as particularly attractive alternatives due to their high theoretical volumetric capacity and potentially lower overall cost relative to existing Li-ion systems. One of the biggest challenges facing the development of multivalent batteries is the fact that the majority of promising electrolytes demonstrated to date are incompatible with either metallic anodes or high voltage cathodes, both of which are required for multivalent systems to compete with existing Li-ion batteries. One emphasis of this program is utilizing electroanalytical techniques in concert with in situ and ex situ spectroscopic probes to develop general descriptors that span working cations (e.g., Ca, Mg, Zn, Cu) in order to create design principles for developing novel multivalent electrolytes. Central to this effort is understanding the role that counter-anions, non-aqueous solvents, and, perhaps most importantly, residual impurities (e.g., H₂O, HF, O₂, etc...), play in modifying the structure of the electrochemical double layer and thus determining the activity, selectivity and stability of multivalent anodes and cathodes.

Equally challenging to the development of functional multivalent batteries is understanding the role of cathode surface structure and (electro)chemistry in guiding the reversible insertion and deinsertion of multivalent ions. In particular, many cathode materials have been predicted to have very high bulk ion mobilities, but in many cases it has proven challenging to access these promising properties experimentally. Through the synthesis of well-defined, single crystalline thin films of candidate cathode materials, we aim to decouple surface phenomena, such as electrolyte decomposition, desolvation barriers, and surface phase transformations, from bulk transport limitations in order to understand, and ultimately mitigate, the bottlenecks that prevent stable and reversible cycling of candidate multivalent cathode materials.

In Situ Characterization of Buried Interfaces in Solid State Batteries

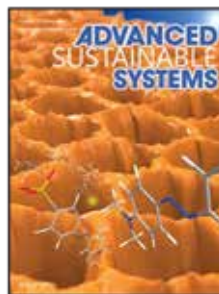
Developing atomic-/molecular-level understanding of the intrinsic (electro)chemical stability of buried interfaces between active materials and electrolytes is critically important to enabling solid-state batteries capable of stable cycling at technologically-relevant energy and power densities. Gaining such insight is complicated by the fact that the relevant interfaces are, by the nature of the cell architecture, inaccessible during cycling, which limits the application of many existing in situ and operando analysis techniques. We have recently developed a surface science-based approach to understand reactivity at buried interfaces in solid-state batteries that applies insights gained from well-defined, model electrode surfaces to understand the resulting performance of real-world materials. This program seeks to understand the influence of surface chemistry, crystallinity and defect content on the intrinsic (electro)chemical stability of solid electrolyte materials in contact with lithium metal and transition metal oxide cathodes in order to develop design principles for synthesizing active and stable interfaces for solid-state batteries.



Seth B. Darling, Ph.D.

Interface Engineering of Membrane and Sorbent Materials

Many applications in water are predicated on specific components from an aqueous fluid either adhering or not adhering to a surface. This principle underlies sensors and sorbents and drives the ubiquitous challenges of fouling and scaling. By manipulating interfacial properties, whether electrostatic, chemical, or structural, it is possible to design highly specific interactions that translate into advantageous performance. One example is to prepare interfaces that tightly bind water molecules in order to create a protective barrier



against attachment of organic or biological species that can nucleate surface fouling. Such passive anti-fouling strategies can be complemented with more aggressive, active anti-fouling approaches by introducing catalytic functionality to water/solid interfaces for self-cleaning operation. For some applications, it may be desirable to selectively adsorb organic molecules to an interface. Marine oil spills are one such application, and our group has done extensive research and development of materials designed for superoleophilicity.

Photothermal Materials for Solar Steam Generation

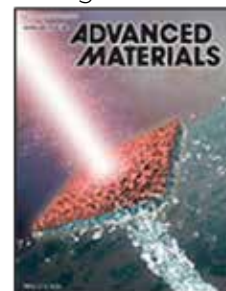
An entirely new way to use membranes has emerged: as photothermal materials for solar steam generation. The goal is to exploit renewable and low-cost energy in the form of sunlight for water evaporation. Distillation has been around for thousands of years, but its implementation has generally involved heating the entire volume of water to drive evaporation. In solar steam generation, in contrast, the object is to localize the thermal energy at the air/water interface, where evaporation takes place. Buoyant porous materials with efficient photothermal conversion properties can achieve this goal. We are investigating a range of different materials for this purpose, with key potential applications in wastewater treatment, desalination and, especially, residuals management.



Isoporous and Janus Membranes for Selective Transport

The vast majority of membranes in use represent materials and technologies developed decades ago with only incremental improvements in their properties and performance since that time. New membrane designs offer the prospect of unprecedented advances in efficiency and function. One such category is Janus membranes, named after the two-faced Roman god because they exhibit different properties on their opposing faces. This architecture enables unique transport phenomena, with wide-ranging potential uses.

Another major challenge with virtually all existing membranes is their broad pore size distribution. Because membranes primarily operate via size-exclusion, having a range of pore sizes forces an operator to select a membrane with an average pore size far smaller than the targeted pollutant in the water to ensure sufficient rejection; this carries an energy penalty and leads to imperfect separations. We are developing methods for scalable fabrication of so-called isoporous membranes. Block copolymer self-assembly provides the templating scaffold, and we have developed methods to transform these materials into nanomeshes with tailored and uniform pores while also providing the option of selecting materials with good thermal, chemical, and fouling resistance.



**Stephan O. Hruszkewycz, Ph.D.****Microscopy of quantum materials with coherent x-rays**

Using x-ray diffraction and microscopy, I am interested in unraveling the relationship between crystal lattice distortions and optical performance in materials such as diamond and silicon carbide that host quantum system. X-rays are particularly well suited for penetrating through sample environments and are very sensitive to subtle changes in a crystal lattice, enabling structural evolution and heterogeneity in materials to be imaged. These methods are based inverting coherent Bragg diffraction, and are particularly powerful for improving materials design of nanoparticles and membranes fabricated for quantum sensing, for observing structural dynamics as a function of time, and for characterizing more speculative quantum material architectures such as hetero-polytype multi-layers in silicon carbide.

Recent related publications:

- Strain annealing of SiC nanoparticles revealed through Bragg coherent diffraction imaging for quantum technologies, Hruszkewycz, et al., Physical Review Materials 2, 086001 (2018). <https://doi.org/10.1103/PhysRevMaterials.2.086001>
- Stabilization of point-defect spin qubits by quantum wells. Ivady, et al., Nature Communications 10, 5607 (2019). <https://doi.org/10.1038/s41467-019-13495-6>

Numerical methods for inverse diffraction problems

My research also encompasses the development of numerical approaches that enable coherent x-ray diffraction microscopy. Coherent Bragg diffraction from a given crystal arrangement can rather simply be modeled, but the inverse problem – the task of determining the crystal arrangement from diffraction measurements – is generally much more difficult. This difficulty stems from the classical “phase problem” in crystallography that has been the subject of research in the field for 100 years. My research group finds novel ways to solve the phase problem in the context of x-ray microscopy of lattice-strain in materials by utilizing modern mathematical optimization and concepts borrowed from deep learning neural networks. These new phase retrieval approaches enable new materials science discoveries by broadening the envelope of possible coherent diffraction imaging experiments.

Recent related publications:

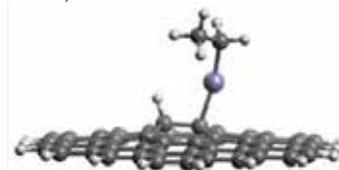
- High-resolution three-dimensional structural microscopy by single-angle Bragg ptychography, Hruszkewycz et al., Nature Materials 16, 244-251 (2017). <http://dx.doi.org/10.1038/nmat4798>
- Measuring three-dimensional strain and structural defects in a single InGaAs nanowire using coherent x-ray multi-angle Bragg projection ptychography, Hill, et al., Nano Letters 18, 811-819 (2018). <https://doi.org/10.1021/acs.nanolett.7b04024>
- Using automatic differentiation as a general framework for ptychographic reconstruction, Kandel, et al., Optics Express 27, 18653 (2019). <https://doi.org/10.1364/OE.27.018653>



Alex B. F. Martinson, Ph.D.

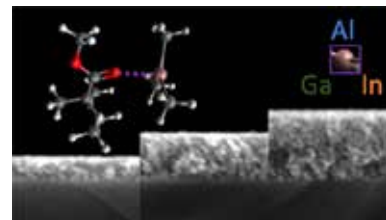
Controlled Atom-Number Clusters for Solar-to-Fuels Catalysis

Few-atom clusters with a narrow distribution of size or even atom-count can exhibit remarkable specific catalytic properties for many energy-related applications including water oxidation. By its nature, atomic layer deposition (ALD) is a digital synthesis route with single-atom resolution that covers the periodic table. However, a lack of control over nucleation and the absence of well-defined interface chemistry hinders the realization of this promising approach. In traditional ALD growth, self-saturating A-B reaction cycles are repeated, the first of which typically nucleates in high density to soon form a thin film. In contrast, we aim to control the nucleation site density and chemistry in order to produce well-separated clusters with prescribed substrate connectivity. This control may be leveraged to improve our command over and understanding of electrochemical reactions of interest, including the oxygen evolution reaction (OER). Our group is exploring multiple platforms for ALD cluster growth including self-assembled monolayers, diamond, and graphene.



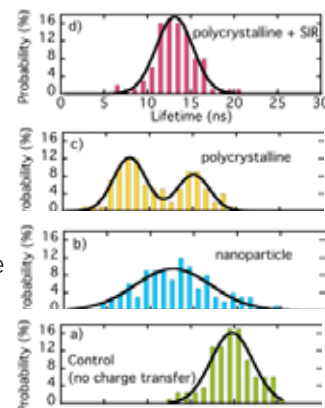
Designer Frameworks for Water Remediation

Our energy economy is intertwined with our water economy on multiple levels, from energy production to energy use in water purification. However, many fundamental challenges remain to understand the complex reactions of aqueous media. For example, the organizational structure of water and its explicit role in catalytic and electrocatalytic processes in confined space at surfaces of solid/liquid interface remains beyond our ability to address experimentally or computationally. We are investigating a range of different materials for this purpose, with key potential applications in wastewater treatment, desalination and residuals management. Sequential infiltration synthesis (SIS), a method derived ALD, enables inorganic hard or hybrid hard/soft materials to be rapidly fabricated from polymer templates with exquisite microstructural organization and complexity. We are expanding the library of materials accessible via SIS processes via novel combinations of polymer class, metal precursors, and process conditions to produce functional isoporous membranes for electrocatalytic processes in confinement.



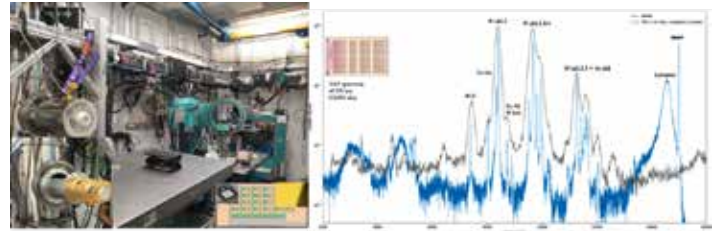
Targeted Surface Synthesis for Electronic Control of Interfaces

Today's most successful thin film synthesis techniques leverage the perfection of single crystalline, atomically smooth, ultrahigh purity, low mis-cut substrates upon which epitaxial growth is performed at high temperature under ultrahigh vacuum. However, the number of materials that can be prepared to such specifications and a shortage of materials that are lattice matched to available single crystal substrates severely restricts our most fundamental understanding of many other materials and interfaces. We are developing the science of selective interface reactions (SIRs), which is an ALD-based approach, to deterministically direct vapor-phase surface reactions chemically tailored so that they selectively modify electronically unfavorable sites of practical (polycrystalline, amorphous, non-lattice matched) materials. For example, SIR treatment of a defective semiconductor surface prior to quantum dot (QD) binding reveals a much narrower distribution of QD lifetimes and therefore charge transfer rates, rivaling that of the intrinsic QD lifetime distribution. We predict, design, and understand selective reaction pathways that can precisely control minority atom arrangements (defects).





Orlando Quaranta, Ph.D.

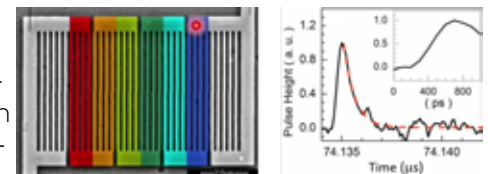


Transition Edge Sensors for X-ray

Modern X-ray science is mostly performed at synchrotrons and free electron lasers due to their ability to provide unmatched photon fluxes, characterized by high degree of stability and coherence, ability to deliver both highly monochromatic and polychromatic beams composed of pulses as short as few ps. These machines allow to gain in depth knowledge of a variety of fields: from combustion engines to microcircuits, development of new pharmaceuticals to pioneering nanotechnologies, and, of course, advanced materials. To make effective use of this potential a suitable set of sensors is needed. The Detectors Group develops a variety of sensors: hybrid pixel detectors, germanium strip detectors, Fast CCD and most recently cryogenics superconducting sensors, such as transition edge sensors (TESs). The underlying motivation for the use of low temperature detectors is the suppression of thermal noise and the ready accessibility of quantum-mechanical phenomena at cryogenic temperatures. Superconductivity is a quantum phenomenon that appears at low temperatures and that plays several important roles in the emergence of low temperature detectors. Superconducting materials are used in sensing elements, sometimes in the supporting cryogenics, and often in the cryogenic read-out circuits that enable sensor arrays. TESs are thermal detectors that rely on the steep resistive transition of a superconducting material as a thermometer and are characterized by energy-resolving capabilities orders of magnitude better than any commercial, semiconductive, sensor. This technology thrives in experiments such as elemental mapping of complex samples, for example to identify different transitional metals used in the production of integrated circuits, X-ray absorption fine structure, where a monochromatic excitation beam is scanned in energy over an elemental absorption edge, proving a measurement of the unoccupied density of states of the element in question, or emission spectroscopy, where the energy distribution of the detected x-rays from a single element at a single excitation energy is used to deduce the occupied density of states of that element which, in turn, is indicative of its chemical environment. The group activity spans from the study of the underlying physics of these devices, to their fabrication and characterization, to finally the deployment of complete instruments at beamlines.

Superconducting Nanowire Single Photon Detectors

A superconducting nanowire single-photon detector (SNSPD) is a single-photon sensor sensitive to a wide range of wavelengths: infrared, visible and X-rays, characterized by with recovery times (ns), timing precision (tens of ps), and dark-counts of orders of magnitude better than any other single photon detector such as single-photon avalanche photodiodes (SPADs) or photomultipliers (PMTs). These advanced detection characteristics make SNSPDs highly attractive for a wide range of applications, such as:



- Quantum key distribution (QKD) - A method for two parties to create a cryptographic key via a public communications channel. This is achieved in practice by encoding information on the phase or polarization of single photons.
- Quantum information science (QIS) - The realization of a quantum computer is undoubtedly one of the grand challenges for physics in the 21st century. One of the key element of this technology is represented by single-photon detectors with near unity detection efficiency and photon number resolving capabilities.
- Characterization of quantum emitters - Single-photon emission from atoms, quantum dots and molecules can be harnessed as a tool for production of quantum states of light for QIS and as a powerful monitoring technique in the life sciences.
- X-ray beam monitoring - The synchrotron radiation can be tuned both in shape (µm size) and in timing (pulses of ps duration at MHz count rate) for different types of experiments.

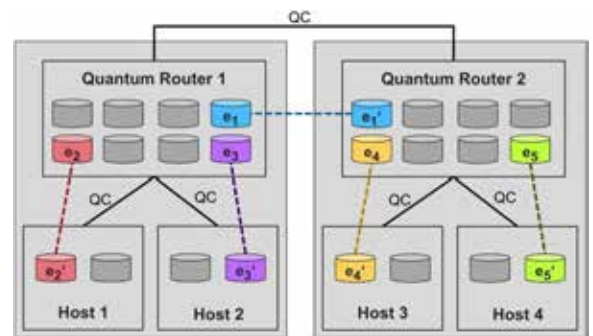
The group has extensive experience in both SNSPD design and characterization and QIS and is actively looking to expand the R&D activity of these devices.



Martin Suchara, Ph.D.

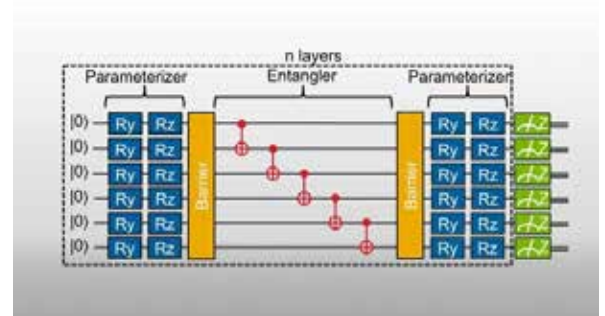
Quantum Communication and Networking

Recent experimental advances make quantum communication networks a reality. The work of our group complements experimental efforts by studying alternative quantum network architectures, designing a suitable control protocol stack, and building a quantum network simulator capable of quickly comparing alternative design choices. Our Simulator of QUantum Network Communication (SeQUeNCe) performs simulations at the individual photon level with picosecond resolution and integrates accurate models of optical components. The challenges we are addressing include overcoming distance limitations of quantum communication, ensuring sufficient scalability and throughput, supporting heterogeneous quantum information sources and applications, and motivating the role of technological advances.



Software Stack for NISQ Architectures

Solving practical computational problems on quantum computers will require new techniques that map large quantum circuits onto systems with limited connectivity and modest qubit counts, as well as mitigating the effects of noise. Our group has been developing quantum circuit compilation methods that, for example, improve efficiency and fidelity by reducing the number of gates and measurement operations in quantum chemistry and molecular dynamics circuits. We have also been developing theoretical techniques and practical algorithms that allow characterizing and mitigating noise inherent in quantum devices. We have been using superconducting quantum processors manufactured by IBM to demonstrate the benefits of our work.



Noisy and Noise-Free Simulation Techniques

Physically motivated simulations of noisy quantum hardware are key to accurate device characterization, providing better understanding of their behavior and more efficient experimental design of these technologies. Noise-free state vector simulations are crucial for benchmarking and understanding the power of quantum computing. We are collaborating with Matthew Otten and Hal Finkel on open quantum system simulations and with the team of Yuri Alexeev and Frederic Chong on noise-free state vector simulations. We develop and implement new techniques to extend the size of systems that can be simulated, such as tensor slicing, matrix product states, and quantum circuit partitioning. We have been using supercomputers at the Argonne Leadership Computing Facility and the University of Chicago Research Computing Center.

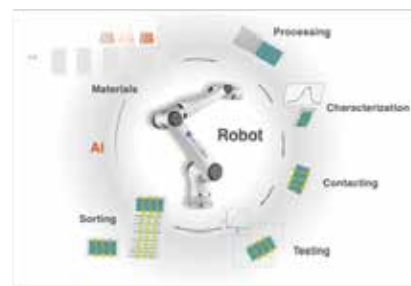




Jie Xu, Ph.D.

AI-guided robotic processing/characterization platform for multifunctional films

A key feature of solution-processed materials - common to a large majority of industrial materials - is that their assembly processes depend on a large number of interrelated processing parameters. A subtle change in one of these parameters can lead to a different molecular packing structure which could drastically influence the properties. Current tedious processing experiments and complex interrelated relationships are planned, operated and analyzed by human scientists and therefore are subject to a variety of human operational/cognitive biases, heuristics and social influences. We are developing a novel approach combining automated robotic machinery, advanced high-throughput processing/characterization and artificial intelligence (AI) data analysis to extract the underlying multi-dimensional processing-morphology-property relationships, quickly identify the paths to the targeted property and reduce human biases.



Engineering Polymer Packing for Printable Electronics/Energy Devices

Controlled assembly of electrically active materials has been a cornerstone to the electronics and energy industries. Recently, the potential to combine mechanical flexibility, low-cost manufacturing (solution-processing) while simultaneously engineering optoelectronic properties has spurred great interest in conjugated polymers. However, it remains a central challenge to control the assembly of such polymers from the molecular to the device scales, which critically impact their performance. We combine advanced printing technology, in-depth morphology and property characterizations to present insights and strategies for controlling the polymer assembly processes, and ultimately, to achieve manufacturing of high-performance novel electronic products and energy devices.



Manipulating Polymer Network for Mechanically Programable Bioelectronics

Seamless and minimally invasive three-dimensional (3D) interpenetration of stretchable electronics within biological structures provide a means for continuous monitoring and manipulation of their properties. Recently developed stretchable electronics can allow for conforming electronics to dynamic and non-planar surfaces, yet targeted delivery of stretchable electronics to internal regions remains difficult. In this research, we are developing tissue-like biocompatible materials with kPa-to-GPa modulus tuning and mechanical actuation. Combined with the intrinsically stretchable electronics we already developed, these new capabilities achieved from this research will greatly advance the bioelectronics, and ultimately, lead to a desirable three-dimensional (3D) continuous monitoring and manipulation on tissue in vivo.

