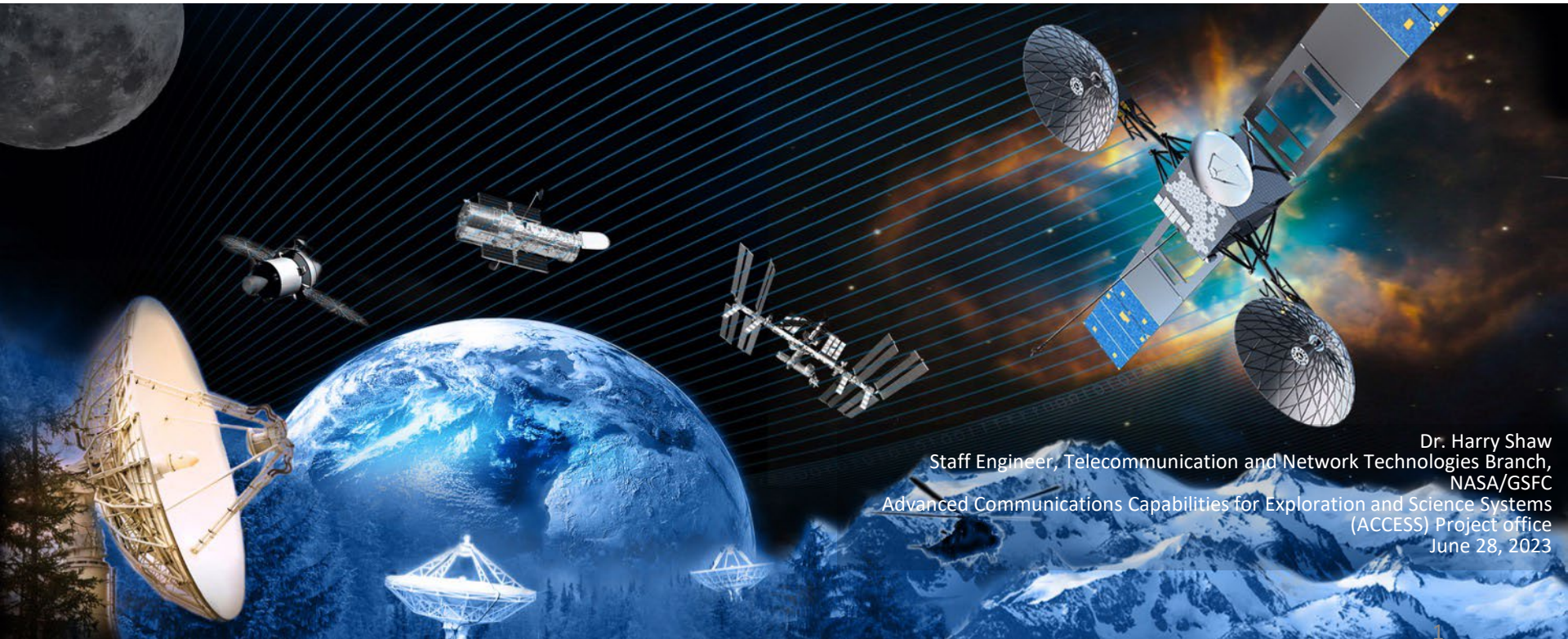




Exploration & **SPACE** Communications

More than you ever imagined...

Virginia Tech Quantum Information Sciences Symposium



Dr. Harry Shaw
Staff Engineer, Telecommunication and Network Technologies Branch,
NASA/GSFC
Advanced Communications Capabilities for Exploration and Science Systems
(ACCESS) Project office
June 28, 2023



- I lead the technical work in quantum research in the Exploration and Space Communications division, Advanced Communications Capabilities for Exploration and Science Systems (ACCESS) Project office at NASA/GSFC along with Dr. Haleh Safavi Our primary focus areas are:
 - Basic and applied research with our partners to support the development of doctorates in quantum-related fields.
 - Some of them will end up within NASA
 - Planning for eventual operations of quantum enabled satellites
 - Improving “quantum literacy” within the American student population with an emphasis on bringing women and underrepresented minorities into the quantum world
 - We have a very robust intern program.
 - We are not full-time researchers. We have “day jobs” operating communications satellites and ground stations

Objectives



- NASA is fortunate to have two former doctoral interns at Virginia Tech
 - Nathan Myers, University of Maryland Baltimore County (Quantum Engines At The Frontiers Of Physics)
 - Kyle Sherbert, University of North Texas (Band Theory And Beyond: Applications Of Quantum Algorithms For Quantum Chemistry)
- NASA/GSFC is interested in continuing collaboration with them and expanding into more areas of mutual interest
- We will provide some background on the work we are currently doing



ACCESS Project Quantum Team



Professional Staff	Degree	Institution	Major
Tyler Williams	M.S	Capitol Technology University	Cyber Security
Alejandro Rodriguez Perez	Ph.D	University of California Irvine	Materials Physics
Deborah Preston	Ph.D	University of California Los Angeles	Chemistry
Erika Jones	Ph.D	George Mason University	Computational Sciences and Informatics
Haleh Safavi	Ph.D	University of Maryland Baltimore County	Electrical Engineering
Harry Shaw	D. Sc.	George Washington University	Electrical Engineering
Robert Lafon	Ph.D	SUNY Stonybrook	Physics
Doctoral Students	Institution	Major	
Manon Bart	Tulane University	Physics	
Naveed Naimipour	University of Illinois Chicago	Electrical Engineering	
Nick Savino	Tulane University	Physics	
Post-doctoral	Institution	Major	
Ian Nodurft	University of Illinois Chicago	Physics	

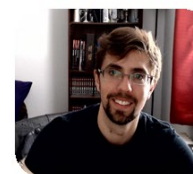
Dr. Deborah Preston

Tyler Williams

Dr. Harry Shaw



Dr. Ian Nodurft



Manon Bart



Naveed Naimipour



Erika Jones

Ph.D

George Mason University

Computational Sciences and Informatics

Haleh Safavi

Ph.D

University of Maryland Baltimore County

Electrical Engineering

Harry Shaw

D. Sc.

George Washington University

Electrical Engineering

Robert Lafon

Ph.D

SUNY Stonybrook

Physics



Dr. Haleh Safavi



Dr. Robert Lafon



Dr. Erika Jones



Nick Savino



Jake Barnes



Dr. Alejandro Rodriguez-Perez



New Mexico State (PI Steven Stochai) – Development of an optical communications testbed



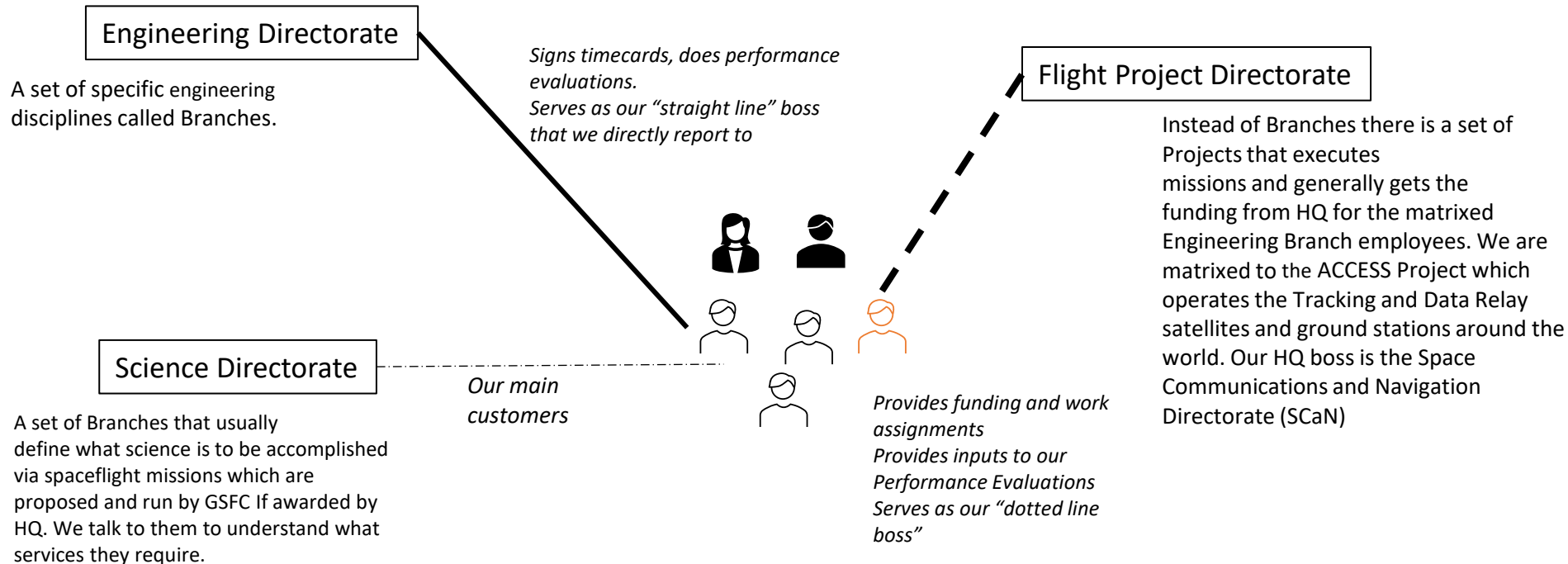
Michigan State (PI Virginia Ayres) - Quantum Demonstration Project



UMBC (PI Sebastian Deffner) – Quantum Thermodynamics

Grants and Subcontracts

A little bit about how GSFC is organized

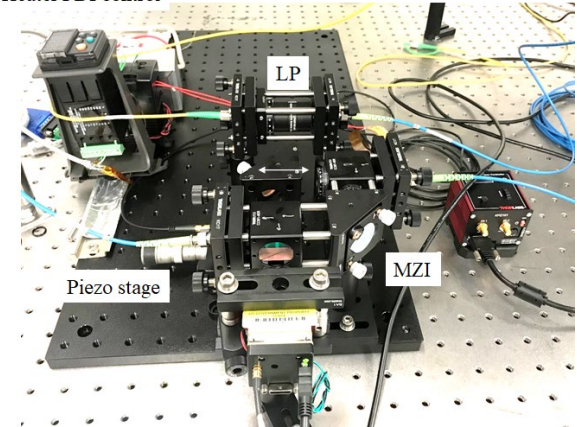


Quantum thermodynamics – Temperature dependence and materials effects in quantum eraser experiments



- Recent Accomplishments
 - Partnership with the Quantum Thermodynamics group at University of Maryland Baltimore County Physics department. PI is Dr. Sebastian Deffner
 - The quantum eraser provides an excellent test bed for a variety of investigations
 - Nathan Myers, granted Ph.D in 2022, Quantum Engines At The Frontiers Of Physics. Now a post-doc at Virginia Tech

Heater PDI control



Aifer, Maxwell, Nathan Myers, and Sebastian Deffner.
 "Thermodynamics of quantum information in noisy polarizers." *arXiv preprint arXiv:2212.00651* (2022).

ACKNOWLEDGMENTS

We would like to thank Todd Pittman, Alejandro Rodriguez Perez, Steve Campbell, and Pat Eblen for enlightening discussions. M.A. gratefully acknowledges support from Harry Shaw of NASA Goddard Space Flight Center. N.M.M. acknowledges support from AFOSR (FA2386-21-1-4081, FA9550-19-1-0272, FA9550-23-1-0034) and ARO (W911NF2210247, W911NF2010013). S.D. acknowledges support from the John Templeton Foundation under Grant No. 62422.

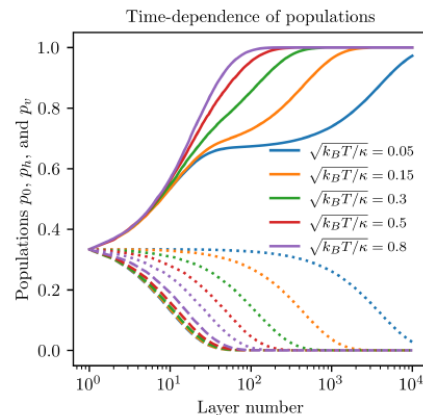
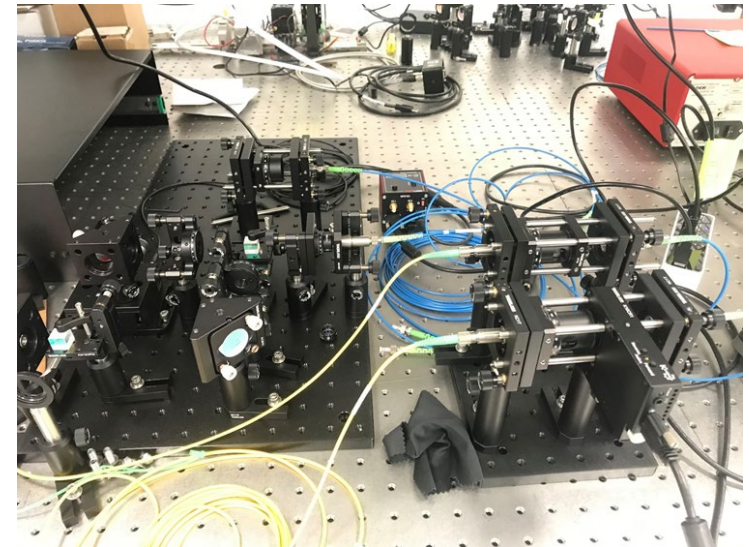


FIG. 7. Populations $p_0 = \rho_{00}$ (solid lines), $p_1 = \rho_{11}$ (dotted lines), and $p_v = \rho_{22}$ (dashed lines). The vertical population p_v rapidly decays to zero but the horizontal component takes longer. As a result the vacuum population has a plateau that is flatter at lower temperatures.



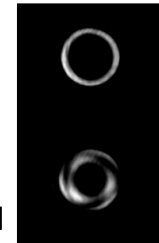
Quantum Communications



Recent Accomplishments:

- Established the first quantum communications laboratory at GSFC
- Baseline quantum entanglement equipment performance of systems at 1550nm and 810 nm
- Conducting experiments in Orbital Angular Momentum for superdense
- Investigating novel materials for propagation and storage of quantum states at $> \text{LN}_2$ temperatures

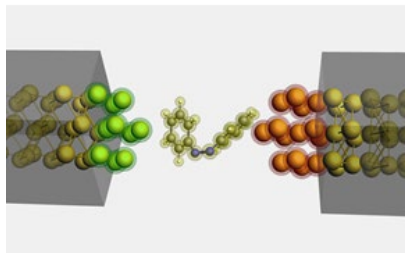
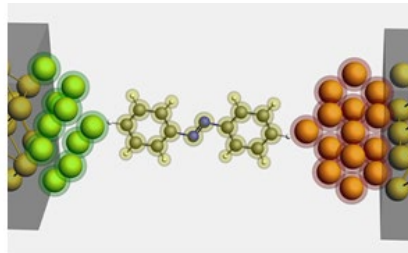
- Photons like other quantum particles contain both spin angular momentum (SAM) and orbital angular momentum (OAM)
- While SAM is relegated to two-dimensional space, OAM belongs to infinite-dimensional space
- OAM modes are orthogonal
 - Allows multiplexing of Classical information
 - Can implement super-dense coding utilizing OAM modes



Partner: Tulane University, Ryan Glasser, PI

Harry Shaw, PI

Quantum chemistry simulation of electronic transport through azobenzene. single molecule circuit simulation



2023 NASA Fundamental Physics Workshop May 23-25, Santa Barbara, California.

Partner: Michigan State University, Virginia Ayres, PI

Hybrid State Effects in Quantum Entanglement Experiments

N. Sebasco¹, J. Vetere¹, G. Panda¹, V.M. Ayres¹ and H.C. Shaw²

¹ Department of Electrical & Computer Engineering, Michigan State University, East Lansing, MI 48824 USA,

²Code 5560, NASA Goddard Space Flight Center, Greenbelt, MD, 20771 USA

Presented

Entanglement in Perovskite Quantum Conductive Layers

G. Panda, N. Sebasco, J. Vetere, V. M. Ayres and H. C. Shaw
Department of Electrical & Computer Engineering, Michigan State University, East Lansing, MI 48824 USA

Code 5560, NASA Goddard Space Flight Center, Greenbelt, MD, 20771 USA

Submitted

Fractalized Quantum Evolutionary Computation

J. Vetere¹, N. Sebasco¹, G. Panda¹, V.M. Ayres¹ and H.C. Shaw²

¹ Department of Electrical & Computer Engineering, Michigan State University, East Lansing, MI 48824 USA,

²Code 5560, NASA Goddard Space Flight Center, Greenbelt, MD, 20771 USA

Submitted



Quantum Computing

Recent accomplishments:

- Established access to the AWS Braket Quantum as a Service. This will allow our quantum algorithms to be tested on actual quantum computers.
- Developed and published approach on quantum compressive sensing

Quantum Compressive Sensing Algorithms

- Built upon algorithms work by Kyle Sherbert (Ph.D Physics 2022, U of North Texas, VT post-doc) & Naveed Naimipour
- Bridging compressive sensing algorithms to quantum computing/communication infrastructure
 - Effects of Shot Noise
- Explored Advantages of Quantum Compressive Sensing
- Key Takeaways



Kyle Sherbert



Naveed Naimipour

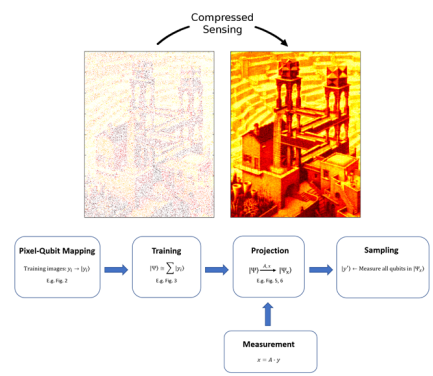
- Basics of quantum computation and circuitry for work on quantum algorithms
 - QISKIT
 - Methods for testing quantum algorithms
 - Built understanding of tomography, noise & quantum noise, compressive sensing techniques

- Implemented a Projection Method for Quantum Phase Estimation

Sherbert, K. M., Naimipour, N., Safavi, H., Shaw, H. C., & Soltanian, M. (2022). Quantum Compressive Sensing: Mathematical Machinery, Quantum Algorithms, and Quantum Circuitry. *Applied Sciences*, 12(15), 7525.

Current and Future Tomography Work

- Exploring post processing areas is integral to the development of quantum tomography
 - Quantum Compressive Sensing
 - Bridging the gap between the quantum and classical worlds of reconstruction
- We present the algorithms and quantum circuits required to implement the training, projection, and sampling steps on a quantum computer
 - We supplement these theoretical results by simulating these circuits with a qualitative model of LIDAR imaging of Earth forests
- Our results indicate that a quantum, data-driven approach to compressive sensing may have significant promise



Amazon Braket Service - Quantum Computing Investigations into Implementing Quantum Compressive Sensing Algorithms

Amazon Braket Features

- “fully managed quantum computing service”
- “build, test, and run quantum algorithms on AWS”
- “access to different types of quantum computers, a unified development environment, a choice of classical circuit simulators, and fully managed execution of hybrid quantum-classical algorithms”

—Amazon Braket Features webpage

NASA Mission Cloud Platform (MCP)

“In collaboration with Amazon Web Services (AWS), MCP provides a consolidated cloud service within NASA, giving mission customers a streamlined process for implementing and using secure, compliant cloud resources.”

Provider	Technology
IonQ	trapped ion — chain of ionized ytterbium atoms where internal states of individual ¹⁷¹ Yb ⁺ serve as qubits and gate operations are via laser pulses to drive two-photon Raman transitions
Oxford Quantum Circuits (OQC)	superconducting — superconducting qubits in 3D (proprietary “Coaxmon”) architecture, i.e., “qubit control electronics perpendicular to the plane of the qubits” [Amazon Braket]
Rigetti	superconducting — “tileable lattices of alternating fixed-frequency and tunable superconducting qubits” [Amazon Braket]
QuEra	neutral atom — arrays of rubidium where internal states of individual Rb atoms serve as qubits, connection of qubits is by Rydberg blockade, and current computational applications target quantum optimization and quantum simulation

GSFC Quantum Communications Lab Plans

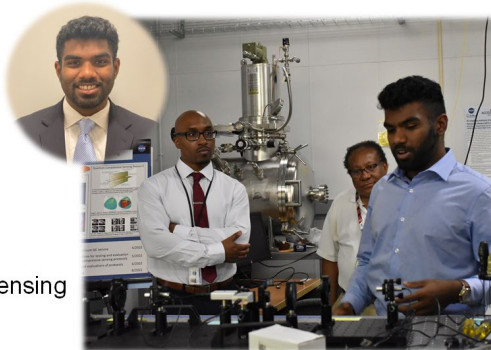
- Use cloud service to run algorithms for quantum compressive sensing protocols
- Access QC technology type of interest for low-cost setup of QC hardware in house

Recent Accomplishments:

- Expanded the intern program to include promising undergraduate students
- Expanding subject matter in the quantum areas

Nishanth Anand

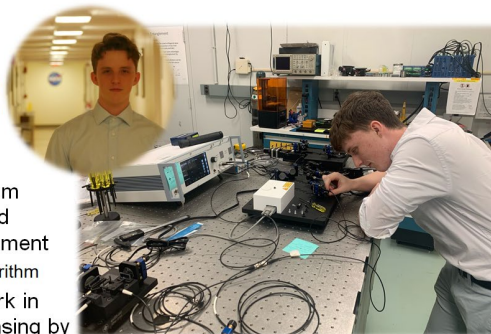
- University of California, Berkeley
- *Bachelor of Arts, Astrophysics / Computer Science, May 2023*



- Performed Experiments
 - QKD with BB84 protocol
 - Quantum Eraser
- Quantum Compressive Sensing Algorithms

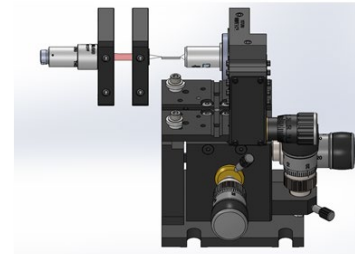
Collin Frink

- University of Wisconsin, Madison
- *Bachelor of Science, AMEP (Applied Math, Engineering, Physics) and Computer Science, December 2022*



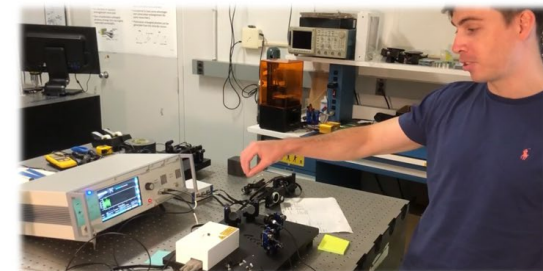
- Trained on low-cost quantum computing tools (Qiskit) and quantum algorithm development
 - Culminated with Shor's algorithm
- Extended previous lab-work in quantum compressive sensing by integrating quantum noise effects

- 2023 NRO Summer Intern Cordell Mazzetti, UT Austin, building a polarization entangled photon source.

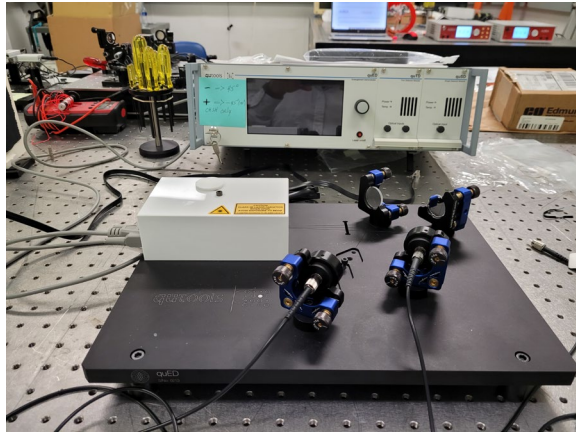


Nick Sebasco

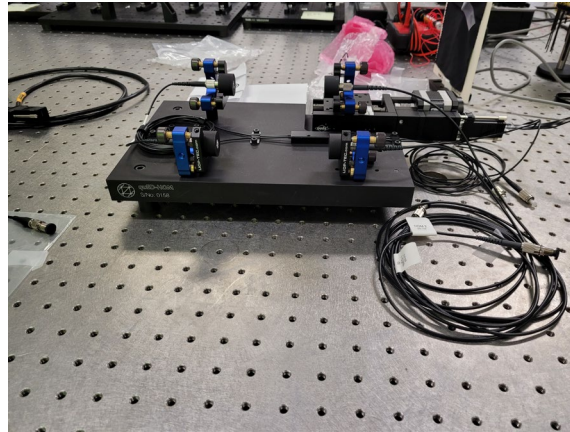
- Developed our Franson Interferometer setup and performed multiple entanglement verification experiments
- Michigan State University
- *MS, Electrical and Computer Engineering, 2023*



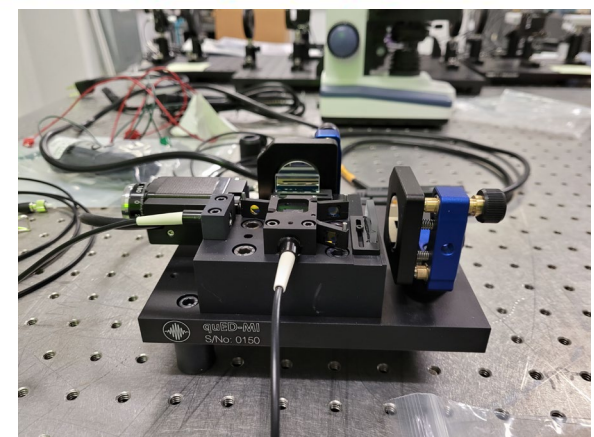
Qutools: This equipment will be used together to perform a variety of experiments



**810nm Polarization
Entanglement System**



Hong-Au-Mandel fixture



Michelson Interferometer

Single Photon Experiments without Interference

Particle Nature of Photons
Quantum Cryptography/QKD: BB84 Protocol
Tomographic Single Photon State Reconstruction
Quantum Random Number Generation

Single Photon Experiments with Interference

Wave Nature of Photons: Single Photon Michelson
Interferometer
Quantum Eraser
Wave-Particle Dualism: Michelson + HBT

Photon Pair Experiments with Polarisation Entanglement

Violation of Bell's Inequality (CHSH)
"Non-Classical" Polarisation Correlations
Tomographic State Reconstruction of an Entangled Photon
State

Quantum Cryptography/QKD: BBM Protocol
Quantum Cryptography: Ekert Protocol

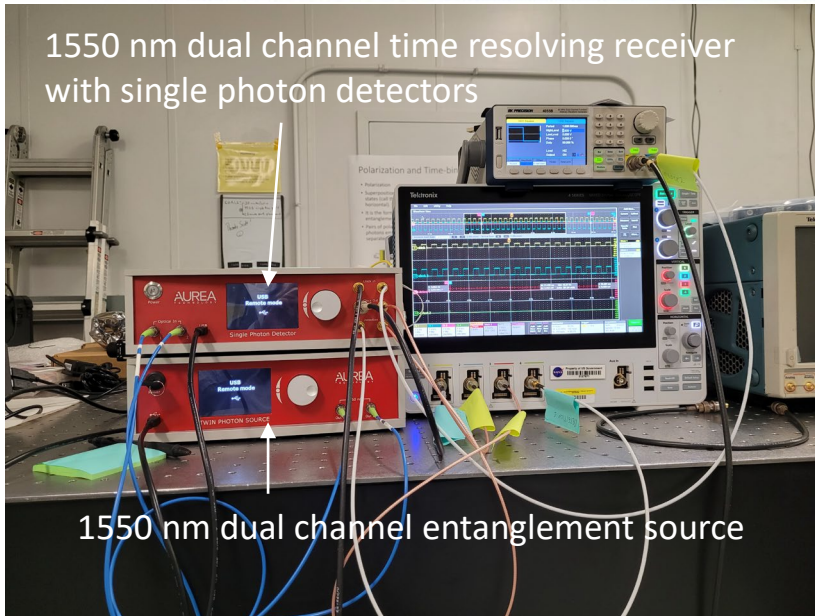
Photon Pair Experiments without Polarisation Entanglement

Hong-Ou-Mandel 2-Photon Interference
Hong-Ou-Mandel Interference + Hanbury Brown & Twiss
Franson Interference

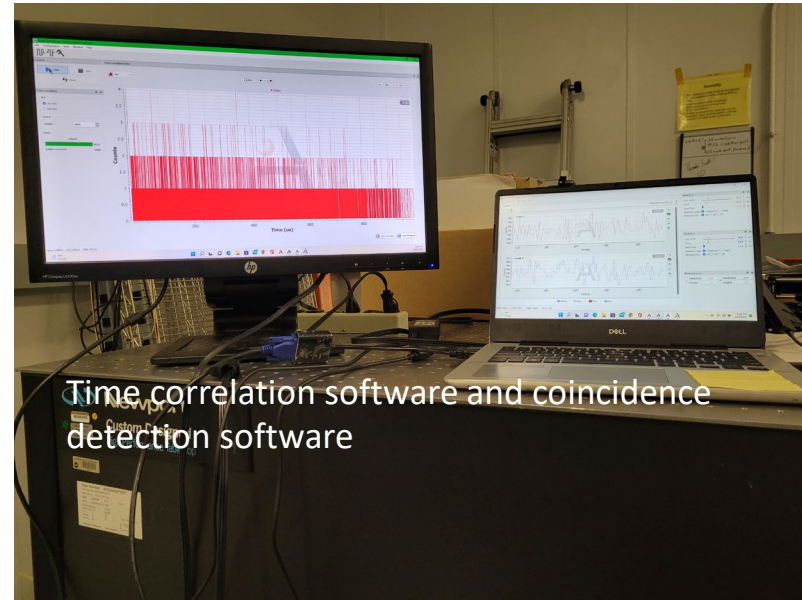
Aurea: This equipment will be used as building blocks for experiments with other equipment



1550 nm dual channel time resolving receiver with single photon detectors

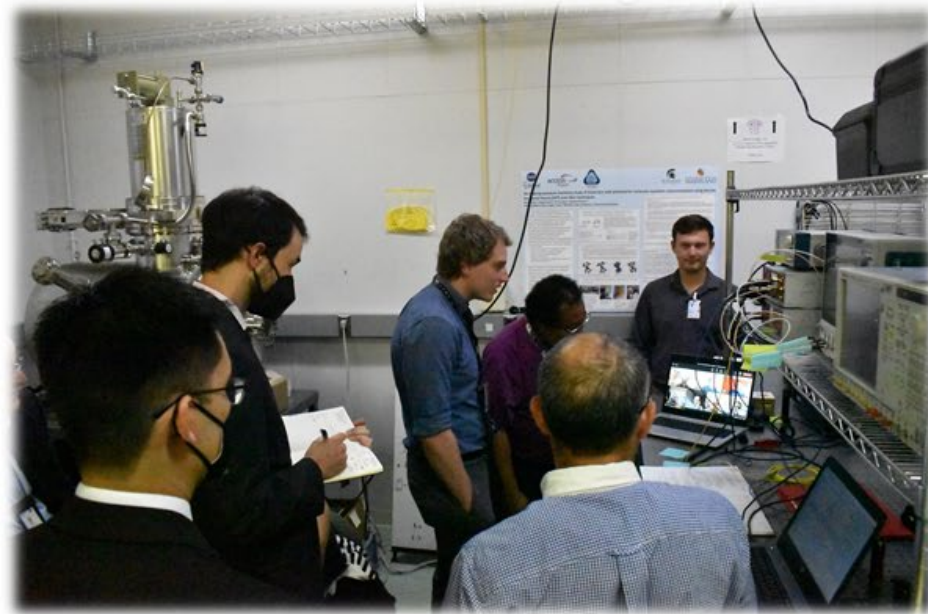


1550 nm dual channel entanglement source



Time correlation software and coincidence detection software

White House Office of Science and Technology, National Quantum Coordination Office visit (August 2022)



OSTP NQCO Drs. Wong and Stambaugh (far left)
with the ACCESS Project Quantum Comm team



ACCESS Project Quantum Comm team
with Dr. Nasser Barghouty (far right)

Summary of main experiments being crafted or in progress



1. Quantum Eraser
2. Fast steering of entangled beams
3. Investigations into entanglement verification and quantum state tomography
 - Clauser-Horne-Shimony-Holt (CHSH) inequality violation
 - Hong-Ou-Mandel (HOM) dip
 - Single Photon Interference with a Michelson interferometer
 - Hanbury-Brown Twiss (HBT) experiment
 - Continue exploring capabilities of our quantum entanglement systems
4. Advancing Orbital Angular Momentum (OAM) investigations towards superdense coding
5. Quantum characterizations of a simulated LCRD downlink
6. Investigations into novel materials for quantum memories and circuits
7. Continue Quantum Compressive Sensing research on LIDAR datasets using Machine Learning
 - Use of commercial quantum computing capabilities to determine the suitability of those capabilities for quantum algorithm solutions
8. Quantum Thermodynamics investigations

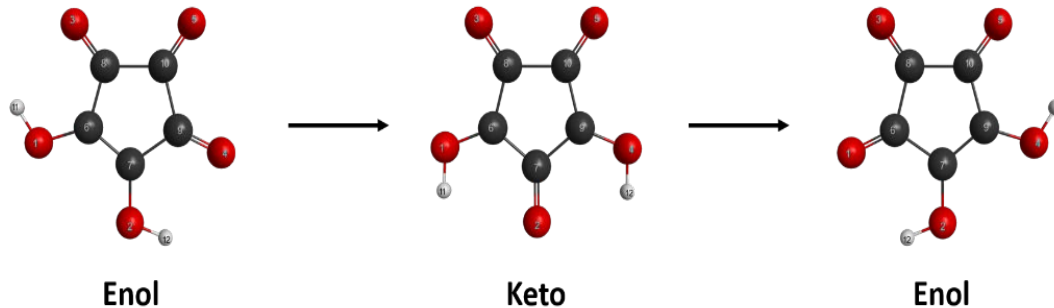
Unpublished Work in Progress



- We have a research project to develop quantum circuits relying on stable tautomeric isomers
- Tautomers are conformational isomers that can take two states
- General questions we are looking at include:
 - Does the transition in states involve a superposition of states?
 - Does it involve quantum entanglement?
 - What is uniquely “quantum” about the circuit implementation?
 - How do we implement these materials in real-world quantum circuits?
- We have two tautomers we are looking at in great detail in simulation
 - Croconic acid
 - Azobenzene

Proton tautomerism in croconic acid

- Croconic acid is an important ferroelectric organic with favorable properties for classical circuits.
- The proton shift certainly provides for a possibility of a quantum oscillator
- There are a number of interesting thermodynamic issues to be explored



Kyle Sherbert's GAMESS simulation

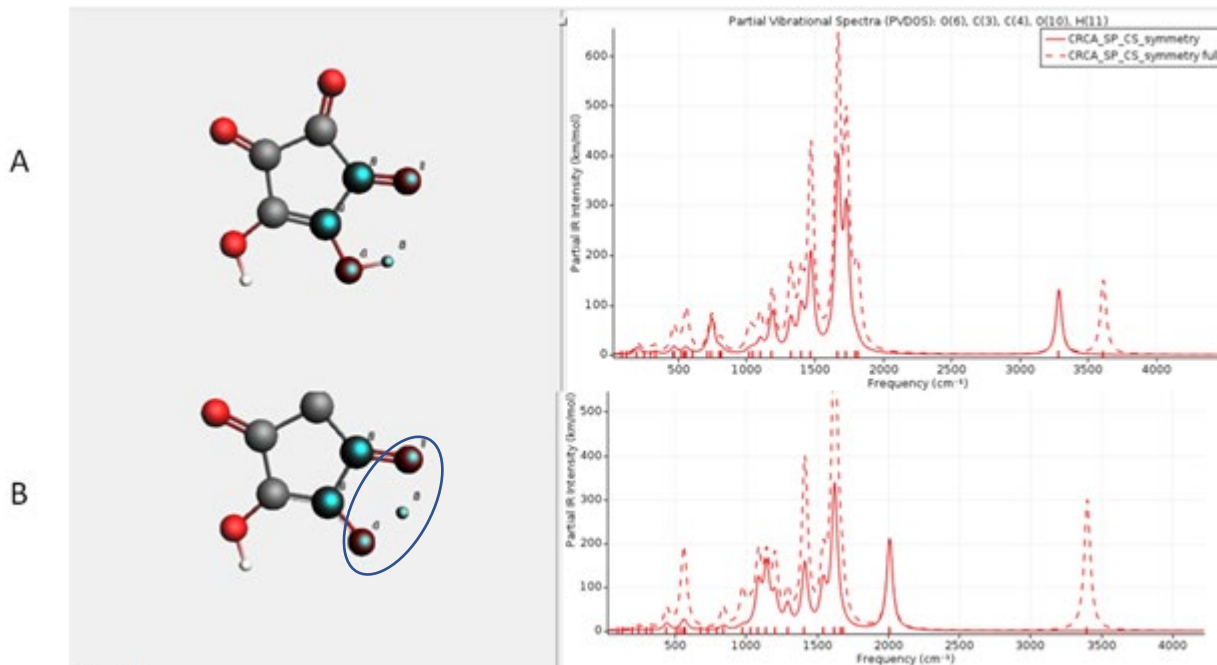
Transition path and the potential energy surface



- We are performing simulations of the transition involving the proton transfer in croconic acid.
- We are using the Amsterdam Modeling Suite (AMS) from SCM and GAMESS
- AMS has a Potential Energy Surface explorer tool
- You define Expeditions and Explorers. They seek out potential energy scans with minimum energy.
- Required multiple iterations
 - 1st iteration: Use many expeditions and a few explorers
 - 2nd iteration. Narrow down candidates from the 1st iteration
 - Speed is tied to the number of cores in the machine. I have 4 cores, so I used only 12 explorers and 50 expeditions the first run and 12 explorers and 8 expeditions for second run

Vibrational spectra and density of states

- Both are important in understanding the mechanisms at work and how we might implement a functioning circuit

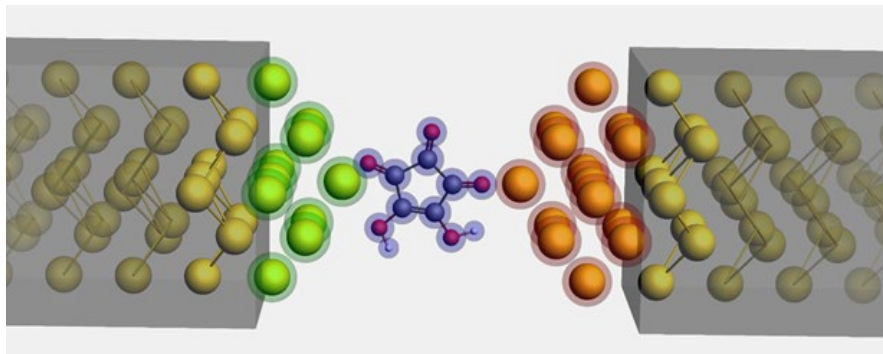


Vibrational spectra of the ground state (A) vs the transition state (B). The stretching mode of H11-O6 (circled) is the single imaginary vibrational mode at -886 cm⁻¹ in the tautomeric transition state. Note the appearance of the peak at 2005 cm⁻¹ in the transition state and the split carbonyl peaks at 3282 cm⁻¹ and 3607 cm⁻¹ in the ground state appear as a single peak at 3395 cm⁻¹ in the transition state.

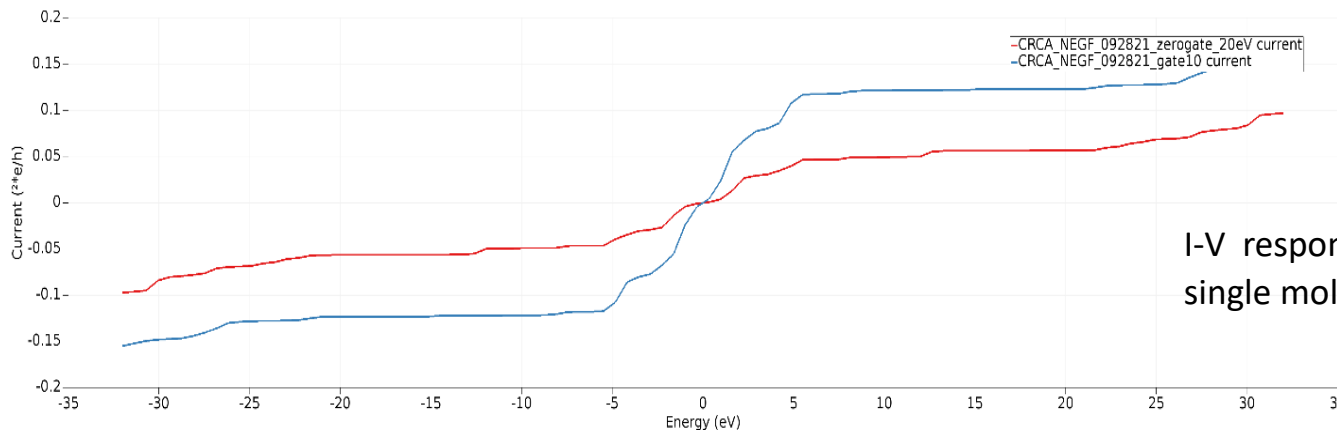
Electronic transport through croconic acid. Single molecule circuit simulation



- AMS uses a non-equilibrium Green's function approach to simulate electron transport
- There is much refinement to be done on these models. We need to include the polarization reversal that occurs under tautomerization. And deep dives into the practical interpretation of the simulation results are to be conducted.
- Additional work is planned to investigate electron and hole mobilities



Single molecule circuit of croconic acid between gold electrodes

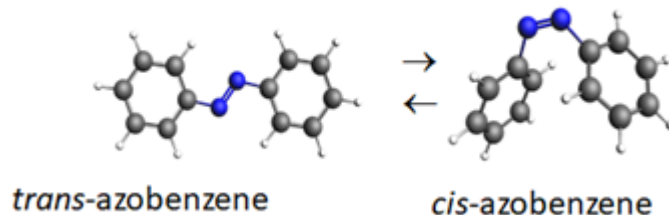


I-V response at zero bias and 10V bias for single molecule croconic acid circuit

cis- & *trans-* tautomerism in azobenzene



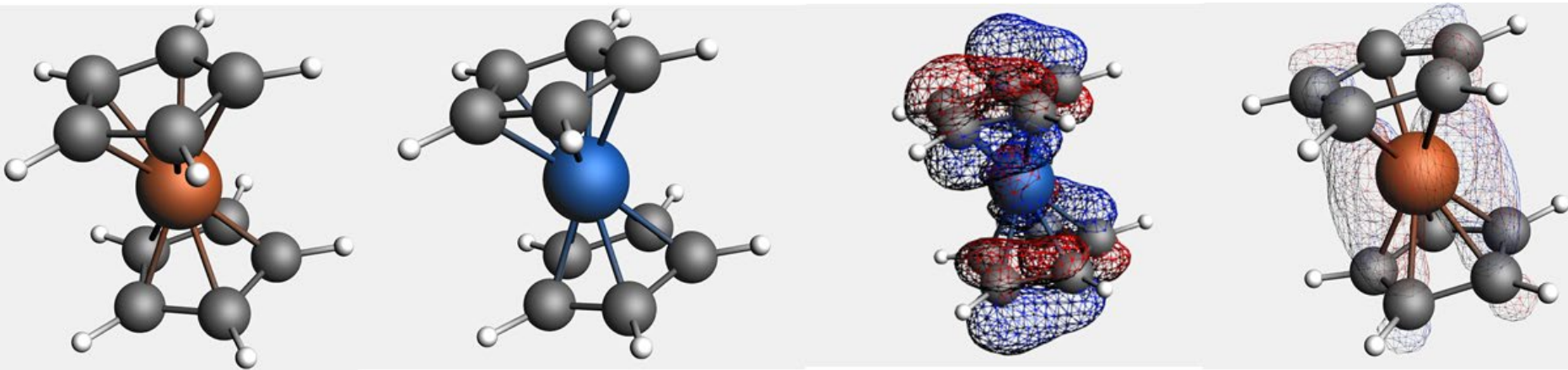
- Azobenzene can be optically stimulated at UV between the ground state (*trans-*) and an excited state (*cis-*) with reasonable thermal stability and reverse switched with visible light
- Azobenzene, and a number of derivatives are also important candidates for classical organic circuit elements such as photoswitches. In our case, we are interested in quantum memories
- We are using AMS modeling suite, GAMESS and ChemOffice which has a good MM2 and MM94 modeling interface



Spin transport through metal cyclopentadienyls



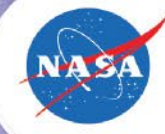
- We are investigating the use metal cyclopentadienyls such as ferrocene and cobaltocene for quantum spin transport
- These molecules are exceeding difficult to model correctly. The highly delocalized nature of the central transitional metal atom to the cyclopentadienyl rings must be accounted for in evaluating the simulation options and results.
- Ferrocene, Cobaltocene and their derivatives are under evaluation with considerations for Aufbau and non-Aufbau⁶ solutions, staggered, eclipsed and skewed configurations, with each constituting a separate symmetry basis



Ground state, Ferrocene and Cobaltocene eclipsed configuration Cobaltocene and Ferrocene HOMO occupations

6. Ghosh, Sayantani, et al. "Entangled quantum state of magnetic dipoles." Nature 425.6953 (2003): 48-51

Sol-gels



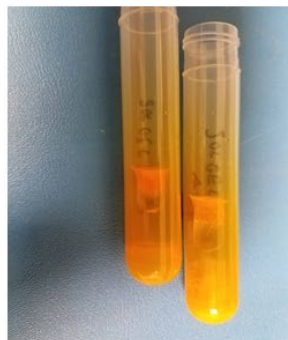
- We have our quantum materials, how are we going to implement them in a practical application?
- Dr. Preston and I are investigating doping silica sol-gel as a substrate.
- We specialize in low temperature synthesis of silica sol-gel and doping them for novel applications ^{8,9}
- Next applications are quantum dots



The sol-gel synthesis process involves acid catalyzed hydrolysis and condensation resulting in polymerization and shrinkage over time. Patience is required to synthesize monoliths.



Mid-cure blank silica sol-gel



Mid-cure azobenzene doped Sol-gel. Note the two phases



3 months later Shrinkage into a Single doped monolith

8. US 6,445,861 B1, 9/3/2002, Sol-Gel Processing To Form Doped, Sol-Gel Monoliths Inside Hollow Core Optical Fiber And Sol-Gel Core Fiber Devices Made Thereby. Harry Shaw, Melanie Ott, Michele Manuel (U of Florida)

9. Preston, Deborah, Jean Claude Pouxviel, Thomas Novinson, William C. Kaska, Bruce Dunn, and Jeffrey I. Zink. "Photochromism of spiropyran in aluminosilicate gels." Journal of Physical Chemistry 94, no. 10 (1990): 4167-4172.



Some other interesting things I've been working on (Ultimately, it's all about communications)

- I have a series of papers using genomics and proteomics for information security which culminated in a patent
- I explore the synergy between molecular biology and information security¹⁰

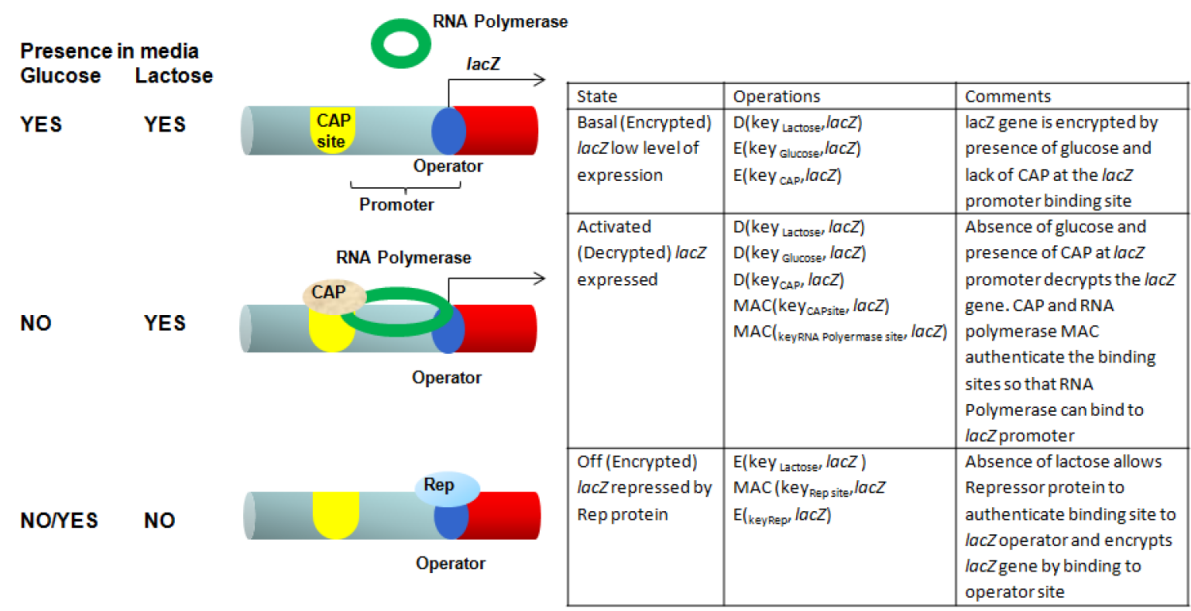
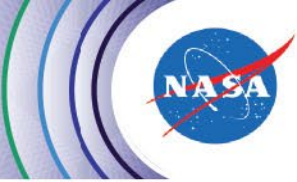


Figure 12. Conceptual example of Confidentiality and Authentication in *E. coli* using *lacZ* expression

10. Shaw, Harry, Sayed Hussein, and Hermann Helgert. "Genomics-based Security Protocols: From Plaintext to Cipherprotein." International Journal on Advances in Security 4, no. LEGNEW-OLDGSFC-GSFC-LN-1046 (2011).



Information theory and signal processing methodology to identify nucleic acid-protein binding sequences in RNA-protein interactions

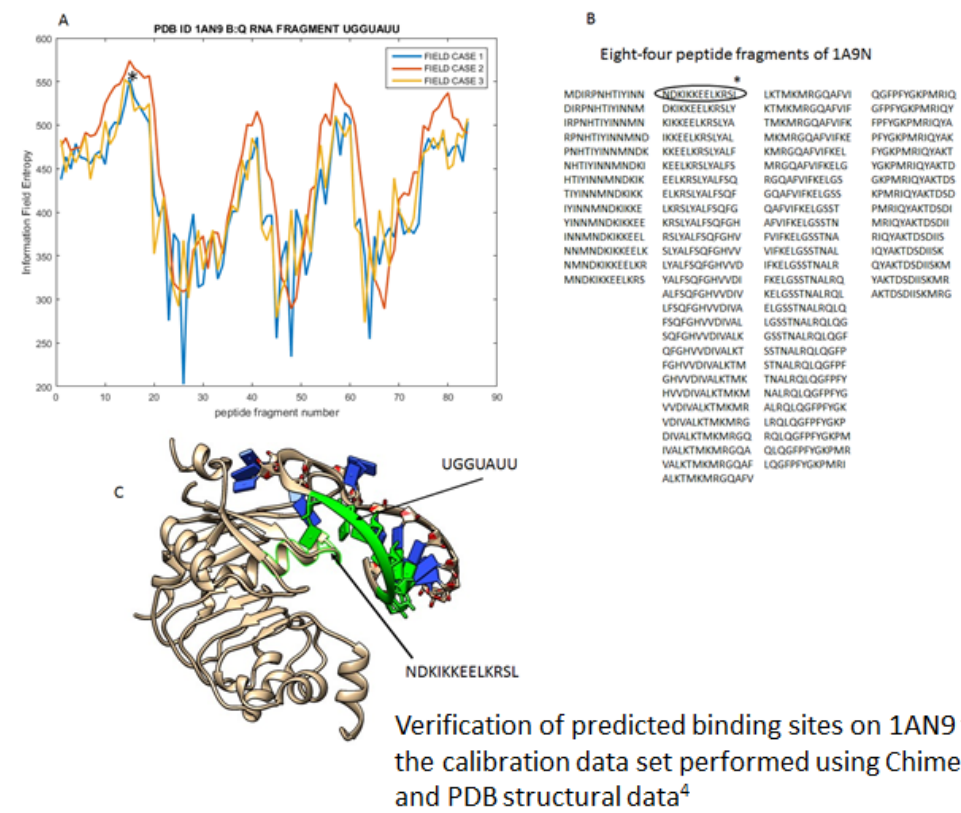
- Harry Shaw^{*}, Nagarajan Pattabiraman^{**}, Deborah Preston[†], Tatiana Ammosova^{††}, Yuri Obukhov^{††}, Sergei Nekhai^{††} and Ajit Kumar^{**}
- ^{*}Telecommunication Networks and Technologies Branch, Staff Engineer, NASA/Goddard Space Flight Center, Greenbelt, MD
- ^{**}Department of Biochemistry and Molecular Medicine, The George Washington University, Washington, DC
- [†]University of Maryland, College Park, MD
- ^{††}Department of Medicine, Howard University School of Medicine, Washington DC

Introduction and Approach



- RNA-protein binding is central to cellular processes
 - Knowledge of the structure of the RNA-protein complex and its formation are key to understanding these processes.
 - In only a fraction of known RNA-protein complexes, structures of bound complexes have been produced using X-ray crystallography or solution NMR.
- The initial goal of this research: predict the binding sites of the microRNA to the each protein using MS/MS assay data.
 - Stretch goal: distinguish the strongly bound microRNA-proteins from the weakly bound microRNA-proteins in the same assay.
- Develop a model that predicts ΔG for RNA-protein binding sites
- Test the model against published RNA-protein binding data. Testing over 200,000 nucleotide:peptide fragments
- The result is an information entropy derived model calibrated against published RNA-protein ΔG for an entire set of assay data.
- Apply to mass spec data from RNA-protein co-immunoprecipitation assays

Produce information field entropy spectra and apply digital signal processing techniques to tease out peaks of interest



PDB ID	total number of predicted matches	total number of predicted matches within 3.5 Å	clash score	Ram outliers	sidechain outliers	RNA backbone	total number of RNA:peptide fragments
1A9N	20	20	C	CD	BC	D	2952
1EC6	16	12	DE	A	D	BC	1050
3AEV	49	33	B	A	D	DE	1035
1SI3	38	22	DE	A	BC	B	411
3R2C	39	21	B	A	BC	DE	816
3K49	30	15	C	B	A	D	1428
1HQ1	9	4	D	E	E	B	3999
2PJP	57	24	D	DE	E	D	1853
2ERR	10	4	AB	C	C	D	97

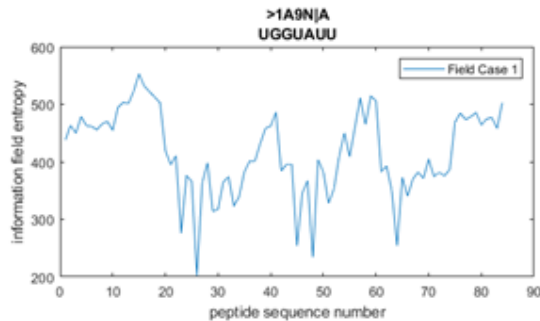
Sample evaluation data. Each entry in calibration dataset underwent a qualitative evaluation of the structure based upon the metrics. The 73 entries were reduced to 30 usable entries based upon this evaluation. A positive hit was registered if one amino acid in the protein segment was within 3.5 Å of any of the nucleotides in the 7 nucleotide RNA segment.

¹⁵Pettersen, Goddard, Huang, Couch, Greenblatt, Meng, Ferrin. J Comput Chem. (2004)
Molecular graphics and analyses performed with the UCSF Chimera package, Resource for Biocomputing, Visualization, and Informatics UCSF

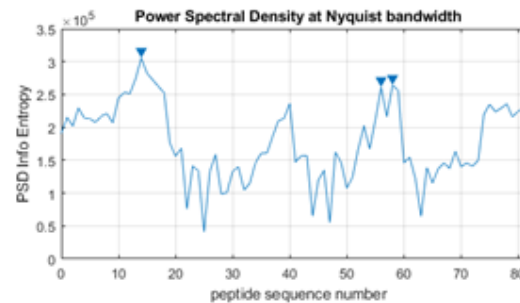
Apply digital signal processing to enhance analysis of peaks



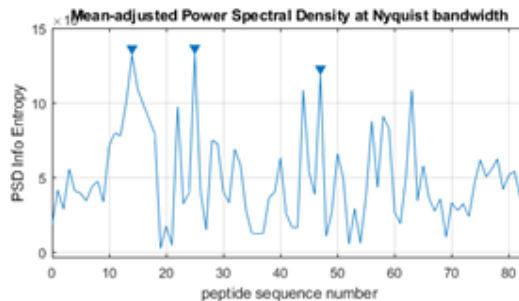
D1



D2



D3



D4

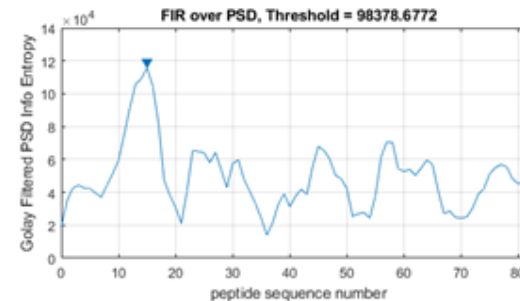


Fig. D represents the results of signal processing the raw spectrum as a time-domain spectrum of the RNA fragment sliding across the protein fragments. Fig. D1 shows the raw information entropy spectra, Fig. D2, D3, and D4 represent successive applications of filtering to enhance location of potential binding peaks.

Connection between quantum entanglement and biochemistry



- It is possible that quantum entanglement in biological systems is more common than originally thought
- NASA is very interested in biomimetic and bio-inspired systems.
 - Biomimetics for NASA Langley Research Center, NASA STTR 2017 Phase I Solicitation, T15.02 Bio-inspired and Biomimetic Technologies and Processes for Earth and Space, Biomimetic strategies for selective carbon dioxide capture with metal-organic frameworks, V.I.N.E. (Virtual Interchange for Nature-inspired Exploration) is a convergence of researchers who are involved in bio-inspired philosophy, sharing tools and research to enable systematic design of nature-inspired systems (GRC)
- It's possible that quantum biochemistry will become an important thrust area for NASA.
- Only researchers with a background in both biochemistry and quantum mechanics, especially the processes of quantum entanglement and the superposition of states will be capable of working in this area
 - Experimental indications of non-classical brain functions, Christian Matthias Kerskens¹ and David López Pérez^{2,1} [Journal of Physics Communications, Volume 6, Number 10](#) *J. Phys. Commun.* 6 105001 DOI 10.1088/2399-6528/ac94be
 - François Fillaux, Quantum entanglement and nonlocal proton transfer dynamics in dimers of formic acid and analogues, Chemical Physics Letters, Volume 408, Issues 4–6, 2005, Pages 302–306, ISSN 0009-2614, <https://doi.org/10.1016/j.cplett.2005.04.069>.

Conclusion



- We are looking for collaboration opportunities with Virginia Tech
- We will cast a wide net.
- We are open to collaboration activities that we have not previously considered