Quantum Chemistry

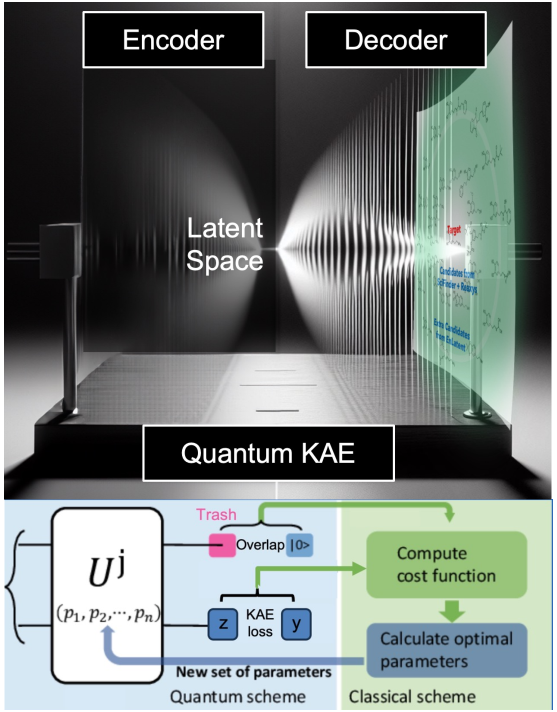
YV 8696: Quantum ML for Retrosynthesis

Background:
Quantum mechanical effects govern many important chemical and biological processes. Batista lab develops computational methods to model the reaction pathways.

Innovation: Kernel autoencoder (KAE) transformer architecture is the first generative approach to retrosynthetic planning (novel synthesis pathway discovery and docking searches).

- Conventional models only use deterministic prediction models.
- Conventional models only encode the reactants. KAE can explore a much larger retrosynthesis space by encoding and decoding the sub-molecular changes.
- Quantum KAE offers exponential data compression on NISQ computing implementation

Use cases; Status:
Yale team has reduced the cost of drug synthesis by 40X for one pharma collaborator.
External validation of an optimized pathway for a commercial herbicide with reduced toxicity.
Yale team has identified improved candidates for a $4Bn approved drug.
Commercial and research user licenses are available. Yale spinout in development to market and support the platform (EnLatent Inc.)



Principal Investigator: Victor Batista

Publication: Kernel AutoEncoder https://arxiv.org/pdf/2310.08685v1.pdf 12 October 2023
Patent: 'Kernel Autoencoder for Template Generative Retrosynthetic Pathways', 2023

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YV 8719: Holographic Computing for Chemistry

Background:
Quantum computing for drug design requires circuits with multiple modes processes. The Batista lab develops Holographic Gaussian Boson Sampling (HGBS) methods to model molecular docking.

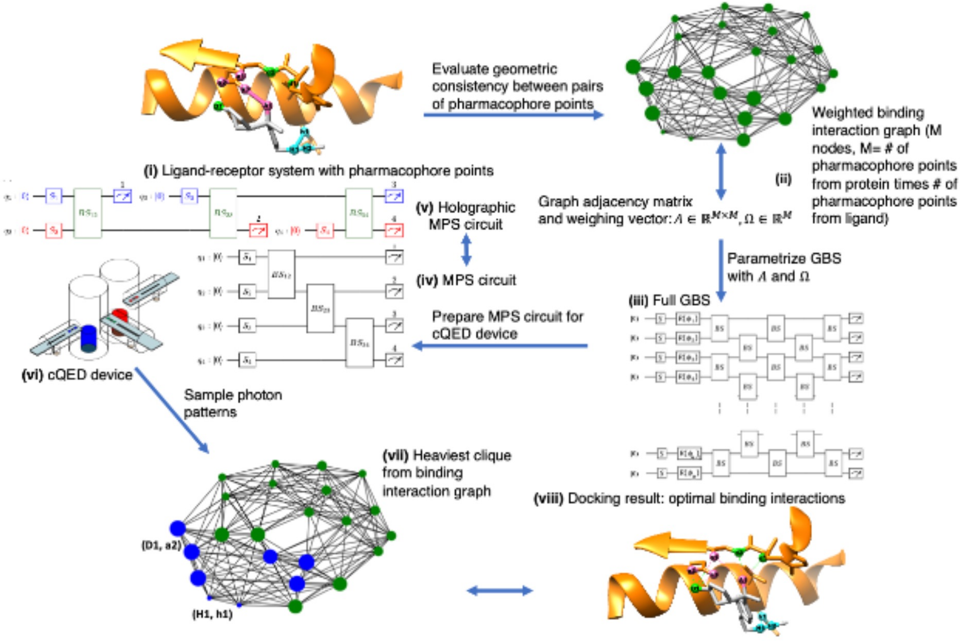
Innovation: The HGBS architecture is the first approach to molecular docking simulations implementable on compact cQED devices.

- Conventional models do not repurpose computational modes.
- Conventional photonic methods use full GBS circuits while HGBS offers data compression in matrix product state (MPS) format.

Use cases; Status:
Yale team has demonstrated HGBS docking simulations of the thiol-containing aryl sulfonamide ligand (see figure, tubes) on the tumor necrosis factor-α converting enzyme receptor (TACE, right figure orange).
Commercial and research user licenses are available. Yale spinout in development to market and support the platform (EnLatent Inc.)

Principal Investigator: Victor Batista
Patent: Holographic Quantum Computing with Bosonic Processors, 2023

Holographic GBS for molecular docking



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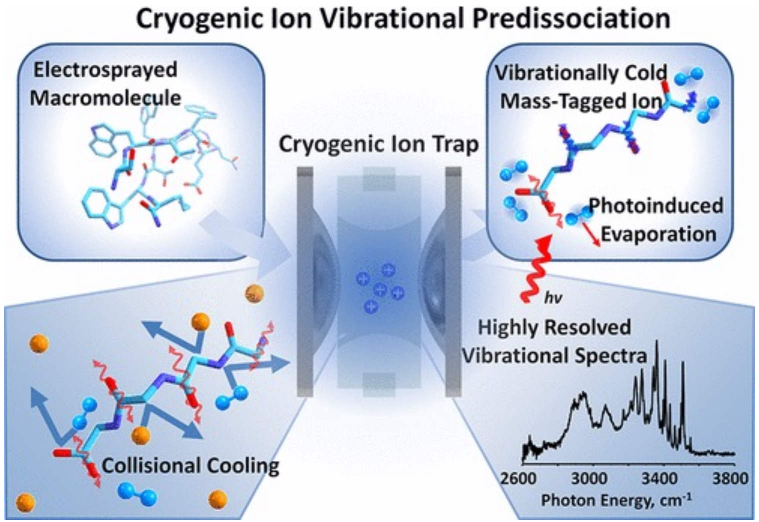
YV 5537: Cryogenic Ion Vibrational Spectroscopy

Background:
Cryogenic ion spectrometry allows for the structural investigation of peptides, labile reaction intermediates, and gaseous cluster ions by isolating transient intermediates via cooling to ~10K in a cryogenic ion trap.

Innovation:
Cryogenic ion traps dramatically expanded the chemical processes which can be resolved with mass spectroscopy, while also increasing the detail of structural information which can be obtained.

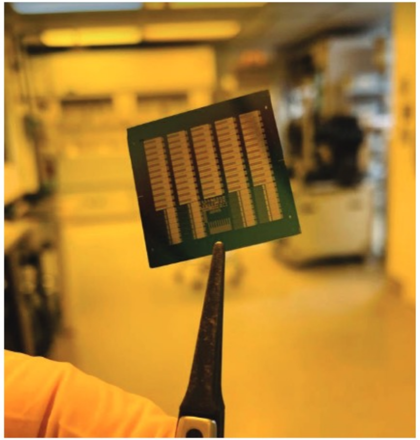
Status/use cases:
- Optimizing catalysts for solar fuel production
- Paired with quantum chemistry, cryogenic ion trap vibrational spectroscopy provides a powerful tool to resolve macromolecular structures and aid in drug discovery.



Principal Investigator: Mark A. Johnson
Publications: Wolk, et. Al., "Cryogenic Ion Chemistry and Spectroscopy." *Acc. Chem. Res.* 2014, 47, 1, 202–210
Publication Date: August 23, 2013. https://doi.org/10.1021/ar400125a
Patent: US Patent 8,890,059

Non-linear Optics

YV 5748: Photon Number Resolving Detectors



Background

- The Tang Lab develops on chip Superconducting Nanowire Single Photon Detectors (SNSPDs) and cryogenic systems for the manipulation and detection of quantum states of light.
- Deep experience with high uniformity manufacturing processes in non-linear optics materials systems AlN, LiNb, NbN.

Innovation: A compact waveguide design for a 100 pixel photon number-resolving chip. Essentially, a CCD chip for quantum uses.

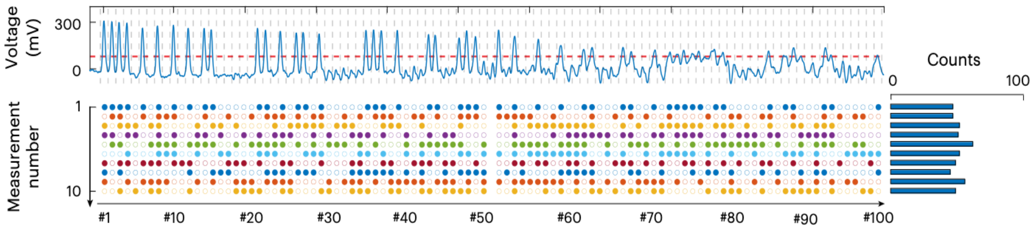
- Features high count rate (sub 1ns time resolution)
- Readout gives POSITION as well as photon number for photon statistics in photon optics experiments.

Use cases; Status

Linear Optical Quantum Computing
Spontaneous Parametric Down Conversion
Improved designs of microwave transmission lines.

Principal Investigator: Hong Tang

Publication: Cheng, R., Zhou, Y., Wang, S. *et al.* A 100-pixel photon-number-resolving detector unveiling photon statistics. *Nat. Photon.* **17**, 112–119 (2023).
Patent: US Patent 9,500,519



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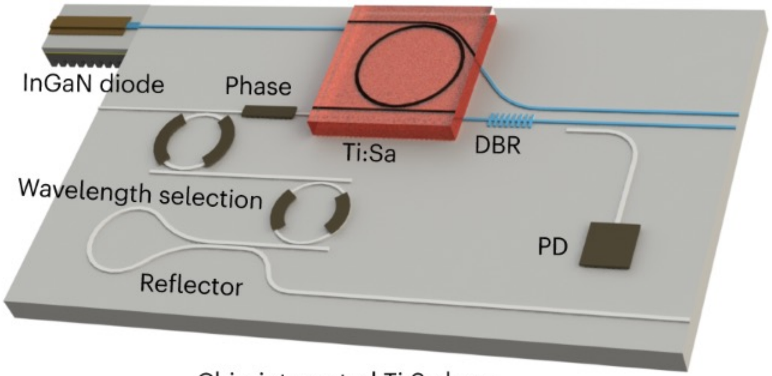
YV 8579: Visible light integrated photonics

Background
- The Tang Lab develops integrated photonics in the visible band which allows chip-scale interface with atomic and trapped ion quantum platforms
- Deep experience with on-chip scalable high uniformity manufacturing processes in non-linear optics materials Al_2O_3, Si_3N_4, AIN, $LiNbO_3$

Innovation:
- Low loss waveguiding < 1dB/cm in the UV-Vis bands
- On-chip Ti:Sapphire lasers

Use cases; Status
Atomic clocks, Quantum atomic-photonic chip technologies, Integrated Light sources, Optical comb technologies.



Chip-integrated Ti:Sa laser

Principal Investigator: Hong Tang

Publication: 15. Y. Wang, J. Holguin-Lerma, M. Vezzoli, Y. Guo, H. X. Tang, “Photonic circuit integrated Titanium Sapphire Laser”, Nature Photonics, 17, 338 (2023).
Patent: 2021 17/166,411 “Octave-Spanning Soliton Comb” and 2023 “TITANIUM:SAPPHIRE (TI:SA) WAFERS, INTEGRATED TI:SA LASERS, AND METHODS OF FORMING THE SAME”
Keywords: Atomic clocks, Frequency combs, Atomic-Photonic chip technologies

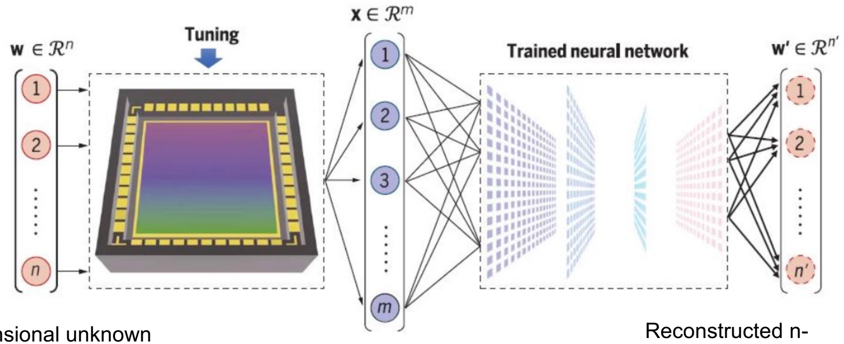
YV 8373: Adaptive Optical Quantum Sensor

Background:
Current optical spectroscopy and sensing platforms are usually non-reconfigurable and do not take advantage of non-linear light-matter interaction properties dominated by quantum geometry.

Innovation:
A new hardware implementation of a transformative learning-based ‘intelligent’ optical sensor that leverages the quantum geometric properties of emerging quantum materials:

- Simultaneous capture of Spectral, Spatial and Polarization Information.
- Maps the physical properties of light using an AI solution.
- Demonstrated reconfigurability at the sensor level.

Use cases; Status
Potential to advance quantum optical sensing to real-world applications.
Yale spinout in development (Deep Optical Sensing Technologies LLC).



n-dimensional unknown optical information

m-dimensional measurement results

Reconstructed n-dimensional information by DNN

Principal Investigator: Fengnian Xia

Publication: Intelligent infrared sensing enabled by tunable Moire quantum geometry, Nature 604, 266 (2022)
Geometric deep optical sensing, Science 379, eade1220 (2023)
Patent: PCT ‘Intelligent Sensing enabled by tunable Moire geometry and quantum geometry’ 2022

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YALE VENTURES

YV 8364: Methods of Fabricating Micro-Mirrors

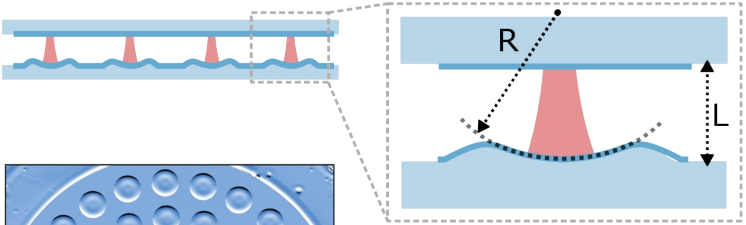
Background: Fabry-Perot (FP) mirrors are highly reflective curved mirrors which may be used to make optical cavities.

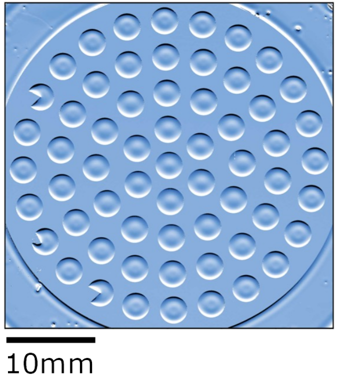
Innovation: Scalable Micro-Mirror Fabrication Process.

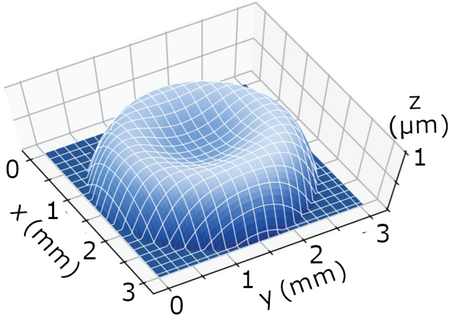
Current micromirror arrays that are prepared using state of the art polishing techniques cannot build the large range of mirror geometries needed for scalable quantum devices and next-generation compact atomic clocks.

- Micro-cavities with finesse > 1Million!
- Range of user-defined curvatures spanning 4 orders magnitude.

Status; Use cases: Full reflow and resist profiling protocol.
Seeking partnerships in neutral atom cavity coupling; quantum optics; frequency metrology technologies; Circuit QED.







Principal Investigator: Peter Rakich

Publications: Jin, et al . Optica 9, no. 9 (2022)
arXiv:2307.08937 (Accepted in Nature)
Patent: PCT/US2023/020253 “MIRRORS, METHODS OF FABRICATING MIRRORS, AND FABRY-PEROT RESONATOR”

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YV 7190: Bulk Acousto-Optic Coupling

Background: In 'acousto-optic coupling', the elastic modes of a crystal structure are engineered to produce efficient coupling of sound and light. Pump light (photons) may be coupled to virtually any transparent structure, producing high frequency coherent acoustic modes (phonons).

Innovation: Rakich lab has identified optimal material treatments to yield world-record (>125 Million) phonon quality Q-factors.

Use cases

- High performance Bulk Acoustic Wave (BAW) resonator demo on-chip.
- Non-invasive laser-based phonon spectroscopy.
- Ideal probe for quantum materials studies.
- Quantum microwave-to-photon modulator.

Principal Investigator: Peter Rakich

Patent: 16/488,223 'Acousto-optic Coupling Techniques and Related Systems and Methods'
https://patentimages.storage.googleapis.com/00/a7/e5/4621ec533aa2f6/US20200030849A1.pdf
Publications: Bulk crystalline optomechanics April 2, 2018 *Nat. Phys.* (published online).https://doi.org/10.1038/s41567-018-0090-3
APL Photonics 3, 066101 (2018) Ultra-high-Q phononic resonators on-chip at cryogenic temperatures May 21, 2018 https://doi.org/10.1063/1.5026798

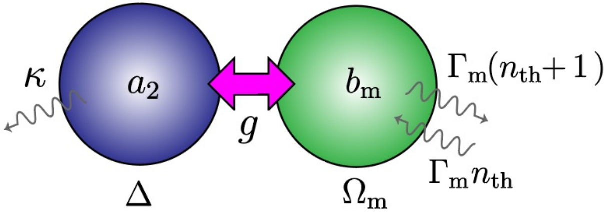

Fig. 1: Strong coupling enables rapid state-swap between photons and phonons

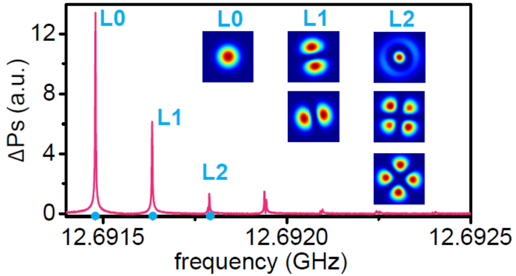

Fig. 2: Phonon Spectrum

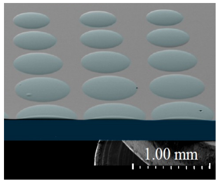

Fig. 3: Phonon array for spectroscopy

Yale

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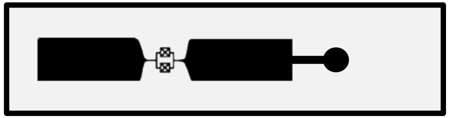
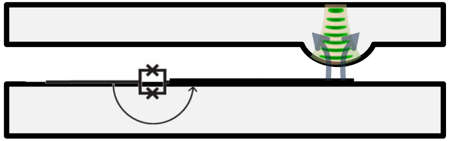
YALE VENTURES

YV 7493: Opto-Acoustic Signal Processing

Background: Exploiting the strong coherent interactions between light and acoustic waves on chip is important for optical communication, microwave photonics, and quantum information transduction.





Innovation:

- A superconducting qubit is piezo-electrically coupled to high-Q phonon mode
- The phonon serves as a quantum memory.
- Built on a wide range of material platforms including aluminum nitride, lithium niobate, silicon and gallium arsenide

Use cases; status:
Prototype Non-reciprocal Interband Brillouin Modulator using Brouillon scattering
Acousto-optic isolators proposed

Fock states: $|1\rangle, \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$, and $|2\rangle$

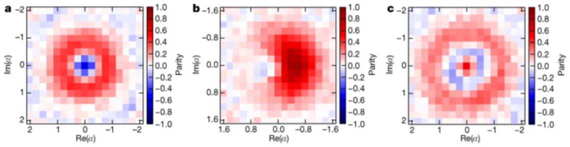


Fig. 1: Non-classical states of mechanical motion

Principal Investigator: Peter Rakich

Patent: US Patant 11,378,741 'Opto-acoustic signal processing'
Publications: Non-reciprocal Interband Brouillon modulation Kharel, APL Photonics (2018); Chu, PTR, Nature (2018)

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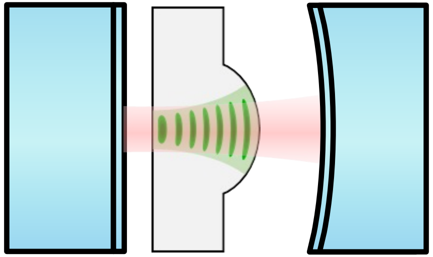
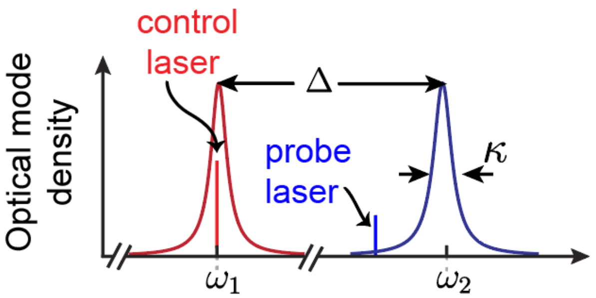
YV 7245: Solid State Optical Quantum Memory

Background: Long lived phonons offer a solid state form of Optical Quantum Memory.



Innovation: Multi-mode acousto-optic waveguide that employs cavity-enhanced Brillouin scattering enables photon-phonon conversion with following advantages over other platforms such as Cesium gas:

- Waveguide integration and design flexibility
- Coupling strength is controlled with laser
- Forward Brouillon scattering so no circulator required, no non-reciprocal devices needed to protect pump light



Use cases; Status:
Enables quantum repeater applications since information encoded in optical photons can be stored and retrieved from phonon mode in Microsecond

Principal Investigator: Peter Rakich

Patent: US Patent 11,101,616 Brillouin Laser
Publication: Kharel, Kharel, "Multimode strong coupling in cavity optomechanics." Physical Review Applied 18.2 (2022).

YV 8101: Atomic Clock Reference Cavity

Background

A Mach–Zehnder Interferometer (MZI) is a device used to determine the relative phase shift variations in quantum sensing and measuring quantum states of light. Optical reference cavities are resonators that provide a way to precisely define an optical frequency for precision metrology and quantum metrology.

Innovation:

- An optical amplifier with reduced residual pump based on MZI

Use cases; Status:

A prototype micro reference cavity for compact atomic clocks which is on the order of 7mm.

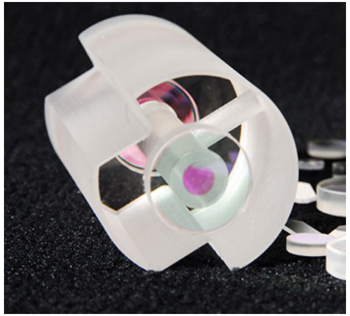


Fig. 1: Conventional Reference Cavity (10 cm)

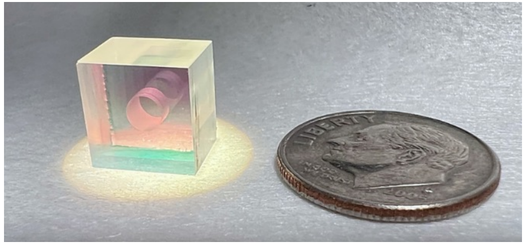


Fig. 2: Yale Micro Reference Cavity (7mm)

Principal Investigator: Peter Rakich

Publications: Jin, et al . Optica 9, no. 9 (2022); arXiv:2307.08937 (Accepted in Nature)
Patent: US Patent 11,652,330 ‘Integrated silicon optical amplifier with reduced residual pump’

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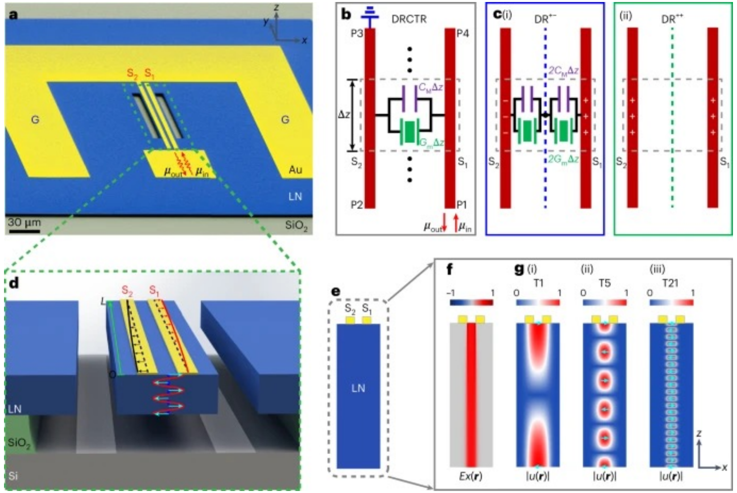
YV 8418: Sub-THz Electromechanical Resonators

Background:
Future 6G communications will require extremely fast data rates, but current state of the art filters (<60GHz) cannot support them. They also cannot act as quantum sensors without cooling to millikelvin temperatures.



Innovation: Sub-THz mm-wave dual rail resonator.
- Breaks the 100 GHz barrier.
- Can maintain a quantum ground state at Kelvin temperatures.
- Based on commercially available thin film LiNb (100nm thickness)
- A suspended LiNb design enables 5 times better performance (higher Q)

Status; Use cases:
Quantum sensor technologies
Extendable to many defense/commercial mm-wave technologies
Enabler for future 6G, but may also be used for current 5G mm-wave band (28GHz) with the same transduction mechanism.

Principal Investigator: Hong Tang

Patent: Patent Application ‘Sub-THz electromechanical Resonators’ 2023
Publication: Nature Electronics March 2023 Sub-terahertz electromechanics, Nature Electronics 6(4):1-6
DOI:10.1038/s41928-023-00942-y

Quantum Computation

YV 8647: Laser Trap for Rydberg Atoms

Background

Circular Rydberg atoms are used long-lived memory applications and neutral atom computing, where the major challenge is decoherence of many-body entangled states.

Conventional traps use a hollow laser to contain the excited atom. The Yale ‘Thread trap' threads or pins a single atom with a laser, offering the following advantages:

- It overcomes the large energy budget of hollow laser traps, which cannot function in a cryostat without a window and high energy losses.
- The trapped Rydberg atom is controllable in a deterministic manner.
- Expected to create stronger long range interactions than field traps/optical tweezers

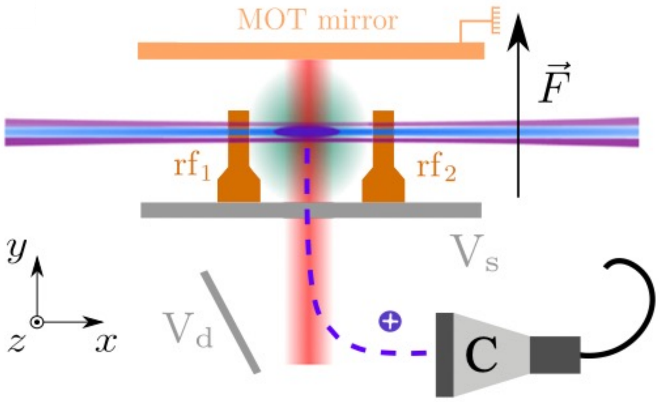


Fig. 1: Rydberg excitation lasers cross in the cold atomic cloud.

Use cases:

Rydberg atoms live 100ms and can be made to live minutes, their states are matched well with long lived memory applications and quantum simulators.
Rydberg Computing companies (Neutral atom platforms), alternative to superconducting circuits, microwave-to-optical conversion at the single atom level.

Principal Investigator: Rodrigo Cortinas

Publications: Laser Trapping of Circular Rydberg Atoms. R. G. Cortiñas. Phys. Rev. Lett. **124**, 123201, 23 March 2020
Patent: Patent Application 'LASER BEAM THREAD TRAP FOR INDIVIDUAL CIRCULAR RYDBERG ATOMS' 2023

YV 8180: Control Engineering for Photonic Cavities

Background:
Cavity resonators, and specifically superconducting microwave cavities, are revolutionizing quantum computation due to long lifetime and fidelity advantages over other platforms. They are also powerful experimental testbeds for quantum error correction and bosonic quantum simulations.

Innovation: A method that engineers the Hamiltonian (target operations in a cavity), by driving an ancilla qubit with an external electromagnetic field.
Advantages include:

- Minimized operation errors
- Delivery of higher complexity operations or quantum simulations
- Design of logical gates that are more resilient to noise

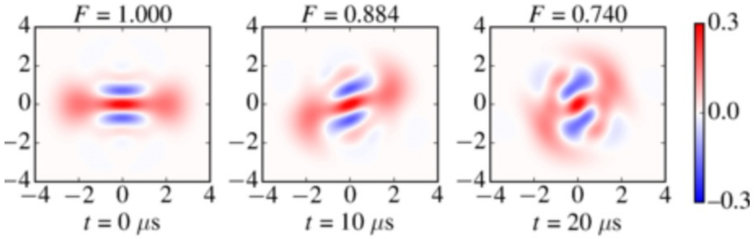


Fig. 1 Simulated evolution of the cavity cat state, energy shifts and gate fidelity.

Use cases; Status:
Transmon qubits and coupled microwave cavities in superconducting circuit systems.
The Yale team has also developed Bosonic Qiskit, a software development toolkit (SDK) extension of the open source Qiskit 2023.

Principal Investigator: L. Jiang, Steve Girvin

Patent: US Patent Application 18/271,370
Publication: Photon-Number-Dependent Hamiltonian Engineering for Cavities Phys. Rev. Applied 15, 044026 – Published 15 April 2021

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YV 8667: Secure Reset for Quantum Computation

Background:
Any entity that gains access to a quantum computer's external electronics, temperature and pulse controller profiles ('Power side channels') and reset operations can exploit them to retrieve certain information about a user's proprietary quantum program and/or to reconstruct the user's circuit.

Innovation: Cascading or Randomized Secure Resets that eliminate information leakage across reset operations.

- Removes risk to multitenancy cloud service providers
- Prevents attackers from using post-reset measurements to recover even part of a pre-reset state.

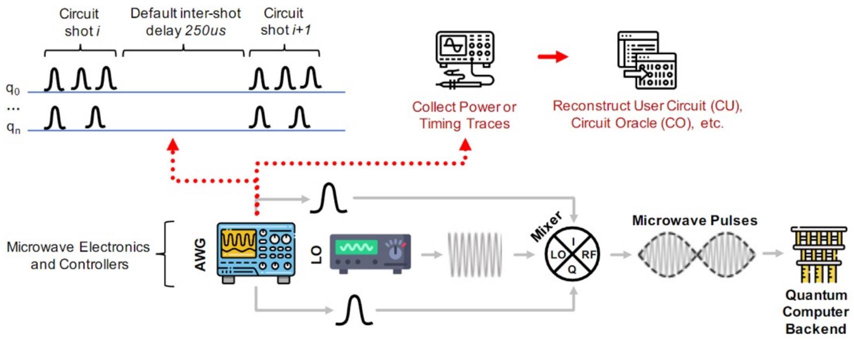

Figure 1. Schematic of a typical qubit drive setup.

Use Cases; Status:
Prototype completed 2023
Seeking benchmarking partnerships with hardware developers.

Principal Investigator: Jakub Szefer

Publication: Extending and Defending Attacks on Reset Operations in Quantum Computers September 12, 2023 https://arxiv.org/pdf/2309.06281.pdf
Patent: Patent Application 'Randomized Secure Resets for Quantum Computers'

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YV 7649: Quantum Random Access Memory QRAM

Background:
The Quantum Computer Systems Lab at Yale (QCSL) builds scalable systems for Noisy Intermediate-Scale Quantum Computers (NISQ) .

Innovation: This Quantum Random Access to Classical Memory (QRACM) allows superposition of addresses (eg. training data for ChatGPT).

- End-to-end system architecture; performs high-fidelity queries of large data sets.
- Avoids the impractical error correction required at each node in a 'bucket-brigade' QRAM design.

Use cases Tailoring quantum algorithms and software to any hardware platform eg. High-level language, Compiler, Runtime, Error correction, Architecture.
Status: Seeking funding, collaborations, commercial partners

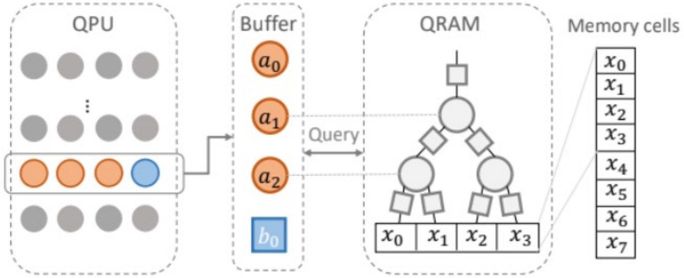

Figure 3: Overview of the proposed virtual QRAM architecture ($k = 1, m = 2$) and its interaction with QPU. The QPU qubits are swapped to the buffer for a quantum query and returned to QPU once the query is done by QRAM.

Principal Investigator: Yongshan Ding

Publications: Systems Architecture for Quantum Random Access Memory. S. Xu, C. T. Hann, B. Foxman, S. M. Girvin and Y. Ding. ArXiv—Published 29 Sep. 2023.\
Textbook: Quantum Computer Systems Research for (NISQ) Noisy Intermediate-Scale Quantum Computers, Y. Din

YV8537: Fast Decoder for Quantum Error Correction

Best Paper Award from IEEE Quantum Computing & Engineering (QCE) 2023.

Innovation:

Fusion Blossom is the fastest known software decoder for *quantum surface codes*. It partitions a decoding problem and can decode a million measurement rounds per second up to a code distance of 33.

- Proven correctness and verified against the Blossom V library with millions of randomized test cases.
- Easy to use interface.

Status: Developing Ultra-low latency QEC decoding (sub-microsecond) with custom hardware (Micro-Blossom).
Hyperion: Towards general *quantum LDPC codes*, beyond surface codes. Seamless correlated decoding when transferring data between qLDPC codes and surface codes.
Yale team is building an extensive library for release in 2024 towards fully error-corrected fault-tolerant quantum computing.

Use cases:

- Any fault-tolerant quantum computer that uses quantum LDPC codes.
- highly accurate minimum-weight decoding for surface codes at microsecond level (with low-latency custom hardware) and other qLDPC codes at millisecond level (with high-end CPUs).
- Seeking partnerships with any lab/company that wants to deploy real-time fault-tolerant control to their quantum computer.

Principal Investigator: Lin Zhong, Yue Wu

Paper: https://arxiv.org/pdf/2305.08307.pdf
Patent: Patent Application "FAST MINIMUM-WEIGHT PERFECT MATCHING (MWPM) DECODER FOR QUANTUM ERROR CORRECTION"

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Quantum Materials

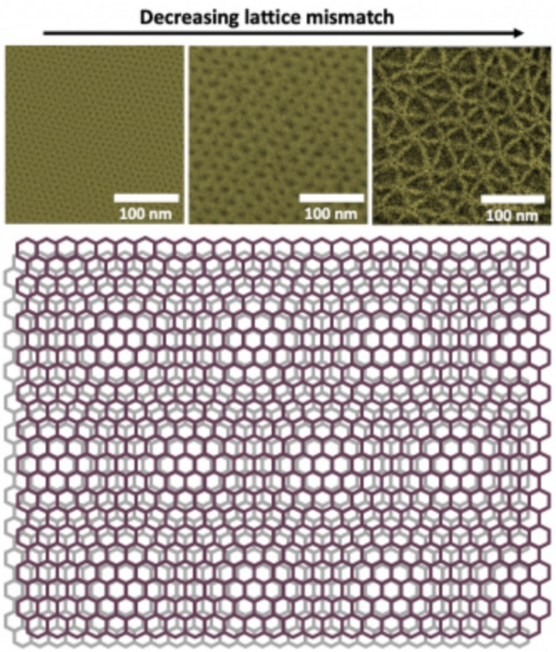
YV 8889: Epitaxial growth of Moiré materials

Background:
Moire superlattices of twisted or lattice-mismatched atomic layers holds great promise for future quantum materials.

Innovation:
Directly grow tunable moire materials by lattice mismatch engineering instead of twisting the layers ‘twistronics’.

- better control, tunability and stability
- may be generalized to 2D magnetic or ferroelectric materials
- scalable if demonstrated on crystalline substrates (eg. Sapphire), currently amorphous substrates only.

Status; use cases:
Van der Waals epitaxy protocols
Demonstrated in WSSe layers (a 2D semiconducting material)



Principal Investigator: Fengnian Xia
Publications: Van der Waals epitaxy of tunable moires enabled by alloying, 14 Aug 2023 Nature Materials 1476-1122