View from Germantown

Advanced Scientific Computing Research Update

Barbara Helland, Associate Director

March 29, 2022

DOE Returns to work

- Re-entry for DOE SC staff began March 14
- For ASCR, most staff will be in the office only 1-2 days a week and telework other days.
  - Tuesdays, Wednesday and Thursday are popular days
- Visitors without HSPD-12 badges need to be escorted
- Masks:
  - Optional when community level is “Low” or “Medium”
  - **EXCEPTION- masks are still required in close quarter indoor environments such as elevators, bathrooms, some shared workspaces, and SCIFs.**
  - Everyone is required to wear masks when community level is “high”
- All Germantown entrances are open, but the Germantown South Gate remains closed
- Germantown Cafeteria is closed for now

ASCR's Computational Partnerships Program Manager

Lali Chatterjee

In January 2022, Dr. Lali Chatterjee joined ASCR as Computational Partnerships Program Manager. Her responsibilities include overseeing SciDAC and Quantum Networking research portfolios in the Research Division. Lali has worked in the Office of Science for over 14 years, starting at ASCR in 2007. She participated in the early stages of the Exascale initiative, oversaw SciDAC partnerships, and started the computational ice sheets research efforts.

Lali comes to ASCR from HEP where she managed the Computational HEP program and accelerated the use of HPC in HEP research and participated in the development of the SC Digital Data Policy. She also created and managed the HEP QIS program 'QuantISED'. Prior to joining DOE, Lali worked as Senior Science Advisor and North American Editor at IOP Publishing and she was in academics - internationally and in the U.S. before that.

Lali is a particle physicist with expertise intersecting nuclear, atomic, molecular, and astro- physics, Her PhD and M. Sc. are from Jadavpur University Kolkata, India and she has over 50 research publications in leading journals.

ASCR Program Manager

Tom Wong

Dr. Tom Wong is an IPA from Creighton University. 20% of the time, he is an ASCR Program Manager in quantum information science, and 80% of the time, he is a detailee at the White House Office of Science and Technology Policy (OSTP) National Quantum Coordination Office.

Tom's research expertise is in quantum algorithms, especially search algorithms involving quantum random walks. Tom graduated from Santa Clara University, triple majoring in physics, computer science, and mathematics and minoring in urban education. He earned a PhD in physics from UC San Diego, followed by two postdocs in computer science at the University of Latvia and the University of Texas at Austin.

Tom has a longstanding interest in education. Between college and graduate school, Tom served as a high school math teacher. He is the author of a free textbook, *Introduction to Classical and Quantum Computing*, whose only prerequisite is trigonometry. He is also the creator of Qubit Touchdown, a football-themed board game that also teaches quantum computing.

More information about Tom is available at thomaswong.net.

New Adventures for Thomas!

Dr. Thomas Ndousse-Fetter retired on December 31, 2021

Thomas received a B.Sc. in electrical engineering from the University of Texas at El Paso, an M. Sc., in computer science from New Mexico Institute of Mining and Technology, and a Ph.D., in George Mason University in respectively. He taught computer science and engineering at Weber state University and at the University of Northern Arizona from 1992 – 1996. He joined the advanced network research group in the Information Technology Lab (ITL) at the National Institute of Standards and Technology (NIST) in 1997 where he worked on optical Internet architectures, protocols, and standards. In 1999, he joined the Office of Advanced Computing Research (ASCR) at the US Department of Energy (DOE) as a R&D program manager responsible for high-performance communication networks and distributed high-end computing. Most recently, he had led ASCR's quantum networking research effort and organized a workshop focused on 6 Ghz wireless networking.

ASCR BUDGET UPDATES

- FY2022 Appropriation
- FY2023 President’s Request

FY2022 Appropriations Language

Office of Science Language:

- The agreement provides not less than $120,000,000 for Artificial Intelligence and Machine Learning capabilities across the Office of Science programs.
- The agreement provides not less than $2,000,000 for collaboration with the National Institutes of Health within the Department's data and computational mission space.
- The agreement provides not less than $245,000,000 for quantum information science, including not less than $120,000,000 for research and $125,000,000 for the five National Quantum Information Science Research Centers.

ASCR Language:

The agreement provides not less than $160,000,000 for the Argonne Leadership Computing Facility, $250,000,000 for the Oak Ridge Leadership Computing Facility, not less than $120,000,000 for the National Energy Research Scientific Computing Center at Lawrence Berkeley National Laboratory, and not less than $90,000,000 for ESnet.

The agreement provides not less than $260,000,000 for Mathematical, Computational, and Computer Sciences Research, including not less than $15,000,000 for computational sciences workforce programs.

The agreement provides not less than $15,000,000 and up to $40,000,000 for the development of AI-optimized emerging memory technology for AI-specialized hardware allowing for new computing capabilities tailored to the demands of artificial intelligence systems.

ASCR Enacted Appropriations
in thousands

	FY2020	FY 2021	FY2022	
	Enacted Approp.	Enacted Approp	Request	Enacted Approp
Mathematical, Computational, and Computer Sciences Research				
Applied Mathematics	41,500	48,570	51,048	51,048
Artificial Intelligence and Big Data (Non Add)	(14,281)	(24,330)	(24,330)	*(24,330)*
Computer Science	38,700	46,827	49,773	49.773
Artificial Intelligence and Big Data (Non Add)	(9,719)	(14,915)	(16,454)	*(16,454)*
Quantum Information Science (Non Add)	(5,000)	(7,256)	(7,256)	(7,256)
Computational Partnerships	69,142	76,194	86,029	79,457
Artificial Intelligence and Big Data (Non Add)	(12,000)	(17,621)	(18,036)	*(19,247)*
Quantum Information Science (Non Add)	(20,680)	(19,209)	(19,209)	*(14,209)*
Research and Evaluation Prototypes	**39,000**	**88,274**	**106,112**	**105,722**
CSGF	**(10,000)**	**(10,000)**	**(15,000)**	***(15,000)***
Quantum Information Science (Non Add)	**(29,000)**	**(71,937)**	**(81,001)**	***(78,021)***
SBIR/STTR	5,658			
Total, Mathematical, Computational, and Computer Sciences Research	155,000	259,865[1]	292,962[1]	286,000[1]
High Performance Computing and Network Facilities				
High Performance Production Computing (NERSC)	110,000	113,786	113,955	118,000
High Performance Production Facility	0	0	2,008	2,000
Leadership Computing Facility at ANL (ALCF)	150,000	152,955	159,047	160,000
Exascale (Non Add)	(150,000)	(150,000)	(150,000)	*(150,000)*
Leadership Computing Facility at ORNL (OLCF)	225,000	228,120	249,066	250,000
Exascale (Non Add)	(125,000)	(120,000)	(125,000)	*(125,000)*
Total, Leadership Computing Facilities	375,000	381,075	381,075	410,000
High Performance Network Facilities and Testbeds (ESnet)	90,000	91,329	93,961	90,000
SBIR/STTR	22,265			
Total, High Performance Computing and Network Facilities	636,265*	586,190[1]	618,037[1]	620,000[1]
Exascale Computing				
17-SC-20 Office of Science Exascale Computing Project (SC-ECP)	188,735	168,945	129,000	129,000
Total, Advanced Scientific Computing Research	**980,000**	**1,015,000**	**1,040,000**	**1,035,000**

[1] SBIR/STTR contained in each activity

*Includes R & E Prototype funds;

FY 2022 Enacted Highlights - ASCR

- Continue the rollout of the fifth cycle of SciDAC to ensure that the teams are equipped to make efficient use of the Nation’s exascale computers.
- Planning to recompete the Mathematical Multifaceted Integrated Capability Centers (MMICC)
- Continue to promote the use of robust AL/ML in scientific simulations and data intensive applications to accelerate scientific discovery.
- Planning to initiate partnerships with other agencies to ensure rapid and robust response to emerging pandemic, biothreat, and public health emergencies.
- Organized a series of workshops in parallel discrete event simulation, cybersecurity and privacy, scientific software development and use, management and storage of scientific data and data visualization to inform its planning for increased investments in applied mathematics and computer science including transitioning ECP efforts back into core research areas.
- Maintained full support, in partnership with the other SC program offices, for the National QIS Research Centers.
- Maintained basic research investments in quantum computing and communications while supporting the quantum computing and quantum internet testbeds to make the exploration of pre-competitive technology accessible to more research communities.

FY2022 Highlights (Continued)

- The ASCR Facilities continue optimal operations delivering high performance computing, storage, and testbed resources to over 10,000 users and high-performance network operations to all DOE national laboratories and dozens of other DOE sites.
- The Facility upgrade projects -ALCF-3 Aurora system, NERSC-9 (Perlmutter) system, and OLCF-5 (Frontier) system- are maintaining their CD-2 baselines.
- The OLCF Frontier system – the Nation's first exascale supercomputer, deployed in Q1 of FY22, is expected to be in-use for early science and ECP applications before the end of the fiscal year.
- The ESnet6 Project is ahead of schedule for anticipated project completion in FY 2022.
- Planning continues for Critical Decision 1 NERSC-10 and the High Performance Data Facility

ASCR: Reaching a New Energy Sciences Workforce (RENEW)

RENEW will:

- **Build foundations** for research and training at institutions historically underrepresented in the SC research portfolio
- **Pilot models of support** that directly address barriers to participation and gaps in the STEM pipeline
- **Evaluate** success and impacts, build on what works.

Based on the outcome of listening sessions with MSIs and the National Strategic Plan for QIST Workforce Development, ASCR will:

- **Organize networking events** to connect DOE labs with potential partners at MSIs (including HBCUs) and other underrepresented institutions
- **Support partnerships** of underserved institutions, national laboratories, and other appropriate partners to**:**
  - Strengthen or establish new quantum computing and networking research collaborations
  - Expand opportunities for undergraduate and graduate students in quantum computing and networking
  - Facilitate access to infrastructure for students to get hands-on lab experience
- **Coordinate** with related efforts sponsored by other agencies such as NSF’s ExpandQISE program (NSF 22-561)

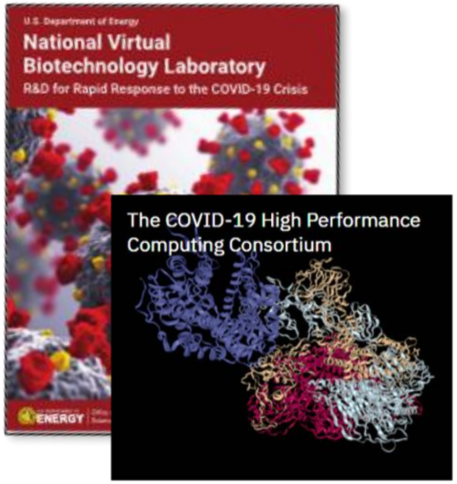
Office of Science's Bio-Prepareness and Response Virtual Roundtable (March 8, 15 & 22, 2022) --BRaVE

Motivation: Considering the impact DOE had through the National Virtual Biotechnology Laboratory (NVBL) and the COVID-19 HPC Consortium, the Roundtable was asked to gather information on unique roles SC can play in **basic science** R&D for future pandemic and related crises.

Goal: Identify priority research opportunities (PROs) and specialized capabilities needed to support biothreat studies at User Facilities.

Topic Areas:

- Surveillance, Testing and Diagnostics
- Molecular Mechanisms, Systems Biology and Therapeutics
- Epidemiology & Event Modeling for Response and Recovery
- Materials and Manufacturing
- Cross-Cutting Issues: Data, AI, HPC and Facilities



Final Report: In progress. Major theme across most areas include data challenges faced over the past 2 years that affected decision making (e.g. access, integration of data streams, federated learning, UQ for decision making). Investments in hybrid infrastructure required that allows data to be efficiently collected, managed, easily and securely accessed across DOE facilities to rapidly meet the challenges of future biothreats.

FY 2023 SC President's Budget Request
(Dollars in thousands)

	FY 2021 Enacted	FY 2022 Enacted	FY 2023 Request	FY 2023 Request vs FY 2022 Enacted		FY 2023 Request vs FY 2021 Enacted	
Advanced Scientific Computing Research (ASCR)	1,015,000	1,035,000	1,068,741	33,741	3.26%	53,741	5.29%
Basic Energy Sciences (BES)	2,245,000	2,308,000	2,420,439	112,439	4.87%	175,439	7.81%
Biological and Environmental Research (BER)	753,000	815,000	903,685	88,685	10.88%	150,685	20.01%
Fusion Energy Sciences Research (FES)	672,000	713,000	723,222	10,222	1.43%	51,222	7.62%
High Energy Physics (HEP)	1,046,000	1,078,000	1,122,020	44,020	4.08%	76,020	7.27%
Nuclear Physics (NP)	713,000	728,000	739,196	11,196	1.54%	26,196	3.67%
Isotope R&D and Production (IRP)	...	82,000	97,451	15,451	18.84%	97,451	...
Accelerator R&D and Production (ARP)	...	18,000	27,436	9,436	52.42%	27,436	...
Workforce Development for Teachers and Scientists (WDTS)	29,000	35,000	41,300	6,300	18.00%	12,300	42.41%
Science Laboratories Infrastructure (SLI)	240,000	291,000	255,000	-36,000	-12.37%	15,000	6.25%
Safeguards and Security (S&S)	121,000	170,000	189,510	19,510	11.48%	68,510	56.62%
Program Direction (PD)	192,000	202,000	211,211	9,211	4.56%	19,211	10.01%
Office of Science	**7,026,000**	**7,475,000**	**7,799,211**	**324,211**	**4.34%**	**773,211**	**11.00%**

FY 2023 Research Initiatives

(B/A in thousands)

	FY 2021 Enacted	FY 2022 Enacted	FY 2023 Request	FY 2023 Request vs FY 2022 Enacted		FY 2023 Request vs FY 2021 Enacted	
New Research Initiatives							
SC Energy Earthshot	...	...	204,250	204,250	...	204,250	...
Funding for Accelerated, Inclusive Research (FAIR)	...	...	35,508	35,508	...	35,508	...
Accelerate Innovations in Emerging Technologies	...	...	40,051	40,051	...	40,051	...
Ongoing Research Initiatives							
Climate and Clean Energy *(includes funding scored to other initiatives)*	2,472,842	2,716,570	3,009,849	293,278	10.80%	537,007	21.72%
Reaching a New Energy Sciences Workforce (RENEW)	...	30,000	60,000	30,000	100.00%	60,000	...
Fundamental Science to Transform Advanced Manufacturing	...	25,353	27,000	1,647	6.50%	27,000	...
Biopreparedness Research Virtual Environment (BRaVE)	...	21,756	51,756	30,000	137.89%	51,756	...
Urban Integrated Field Laboratory	...	17,000	22,000	5,000	29.41%	22,000	...
National Virtual Climate Laboratory (NVCL)	...	3,000	3,000	...	...	3,000	...
Climate Resilience Centers	...	5,000	5,000	...	...	5,000	...
Microelectronics	30,182	47,701	47,701	...	...	17,519	58.04%
Critical Materials/Minerals	17,000	25,000	25,000	...	...	8,000	47.06%
Quantum Information Science	270,391	293,075	293,426	351	0.12%	23,035	8.52%
Artificial Intelligence and Machine Learning	124,354	129,837	169,000	39,163	30.16%	44,646	35.90%
Exascale Computing	479,945	445,000	268,000	-177,000	-39.78%	-211,945	-44.16%
Revolutionizing Polymers Upcycling	14,500	14,500	14,500	...	...	...	...
Accelerator Science and Technology Initiative	11,411	34,725	28,872	-5,853	-16.86%	17,461	153.02%
Advanced Computing *(formerly Integrated Computational & Data Infrastructure)*	11,974	32,657	37,661	5,004	15.32%	25,687	214.52%
Total, Research Initiatives	**3,432,599**	**3,841,174**	**4,342,574**	**501,399**	**13.05%**	**909,975**	**26.51%**

SC Energy Earthshots Initiative
FY 2023 $204M

- Accelerates breakthroughs to realize abundant, affordable, and reliable clean energy solutions within the decade
- Addresses key research challenges at the interface of basic and applied research to bridge the R&D gap
- Initiates new research modality, Energy Earthshot Research Centers (EERCs)
  - Advances foundational knowledge and state-of-the-art capabilities in experimental, theoretical, and computational sciences needed to realize new approaches and solutions
  - Brings together large, multi-investigator, multi-disciplinary teams
  - Coordinates closely with the Energy Technology Offices and existing research consortia/demonstration projects for a new era of cross-office research cooperation
- EERCs will be complemented by small group awards focused on use-inspired fundamental research to address knowledge gaps that limit achievement of the Energy Earthshot goals

Hydrogen Shot

<100 Dollars

1 Ton

1 Decade

Long Duration Storage

Reduce storage costs by **90%***…

…in storage systems That deliver **10+** hours of duration

…in **1** decade

*from a 2020 Li-Ion baseline

Carbon Negative Shot

1 Dollar

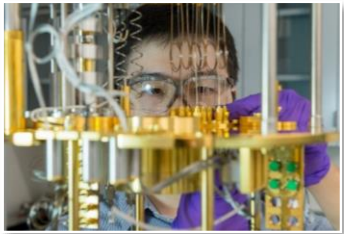
1 Kilogram

1 Decade

Funding to Accelerate Inclusive Research (FAIR)
FY 2023 $36M

FAIR will enhance research on clean energy, climate, and related topics at minority serving institutions (MSIs), including underserved and environmental justice regions

- Builds research capacity, infrastructure, and expertise at MSIs
- Develops mutually beneficial relationships between MSIs and DOE national laboratories and user facilities
- Complements the RENEW initiative (internships at national laboratories for workforce development)
- Provides support of single PI or research teams, and includes an equipment or infrastructure element
- Majority of funds will go directly to HBCUs/MSIs, a portion will fund the partnering institution (Lab, university)

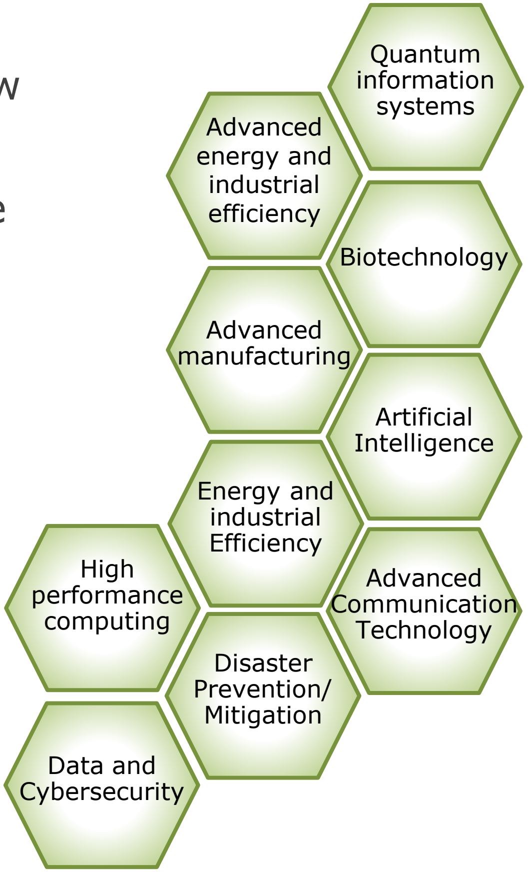


Accelerate Innovations in Emerging Technologies
FY 2023 $40M

Initiative goals:

- To drive scientific discovery for sustainable production of new technologies across the innovation continuum
- To train a STEM workforce to support industries of the future
- To meet the nation’s needs for abundant clean energy, a sustainable environment, and national security

Highly integrated research teams to accelerate the discovery, creation, production, and commercialization of new technologies to form the basis of future industries with public and economic impact



U.S. DEPARTMENT OF ENERGY | Office of Science

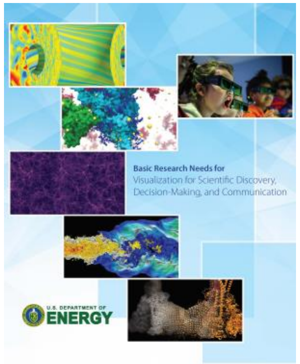
ASCR - FY 2023 President's Request

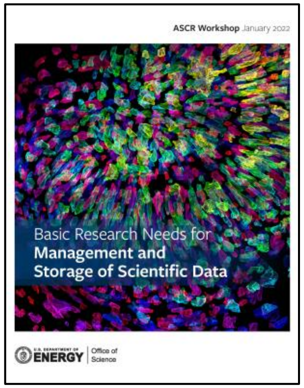
(Dollars in thousands)

	FY 2021 Enacted	FY 2022 Enacted	FY 2023 Request	FY 2023 Request vs FY 2022 Enacted		FY 2023 Request vs FY 2021 Enacted	
Advanced Scientific Computing Research							
Applied Mathematics Research	48,570	51,048	71,938	20,890	40.92%	23,368	48.11%
Computer Sciences Research	46,827	49,773	70,326	20,553	41.29%	23,499	50.18%
Computational Partnerships	76,194	79,456	97,861	18,405	23.16%	21,667	28.44%
Advanced Computing Research	88,274	105,723	113,598	7,875	7.45%	25,324	28.69%
Energy Earthshot Research Centers	...	...	25,000	25,000	...	25,000	...
Mathematical, Computational, and Computer Sciences Research	**259,865**	**286,000**	**378,723**	**92,723**	**32.42%**	**118,858**	**45.74%**
High Performance Production Computing	113,786	120,000	115,033	-4,967	-4.14%	1,247	1.10%
Leadership Computing Facilities	381,075	410,000	407,772	-2,228	-0.54%	26,697	7.01%
High Performance Network Facilities and Testbeds	91,329	90,000	90,213	213	0.24%	-1,116	-1.22%
High Performance Computing and Network Facilities	**586,190**	**620,000**	**613,018**	**-6,982**	**-1.13%**	**26,828**	**4.58%**
17-SC-20 SC Exascale Computing Project	**168,945**	**129,000**	**77,000**	**-52,000**	**-40.31%**	**-91,945**	**-54.42%**
Total Advanced Scientific Computing Research	**1,015,000**	**1,035,000**	**1,068,741**	**33,741**	**3.26%**	**53,741**	**5.29%**

FY 2023 Request: ASCR Research

- The Request prioritizes foundational research across ASCR to transition and sustainment of critical technologies from the ECP, ensuring that ASCR continues to meet SC's HPC mission needs during and after the Exascale Computing Project (ECP) final deployment.
- Investments in core research will continue to address the combined challenges of increasingly heterogeneous architectures and the changing ways in which HPC systems and data storage will be used, the development of new scalable energy efficient algorithms and software and new data management and visualization techniques and tools to understand uncertainty and complex scientific data.
- Provides an increase **(+$13M)** to continue the incorporation of AI and ML into simulations and data intensive applications while increasing greater connectivity with distributed resources, particularly at other SC user facilities through development of new workflows and storage techniques from the device to HPC.
- The increase also supports continued efforts to actively build workflows that ensure rapid and robust response to emerging pandemic, biothreat, and public health emergencies and partnership with the National Cancer Institute **(+$6M)**
- ASCR will maintain full for the National QIS Research Centers, basic research investments in quantum computing and communications and in quantum computing and quantum internet testbeds.





FY 2023 Requests: New Initiatives

- **EARTHSHOTS (+50M): ASCR will partner with BES and BER to**
  - Establish Energy Earthshot Research Centers to create large, multi-investigator, multi-disciplinary teams in coordination with the applied technology offices
  - Invest in small group awards in applied math and computer science that focus on incorporating AI/ML in use-inspired fundamental research to support the Department's Earthshots.

- Increases investments to broaden participation in ASCR research and education programs by under-represented groups.
  - **FAIR (+4M)** –to compliment our RENEW and ECP efforts, **ASCR** will invest in midrange equipment to broaden participation in ASCR quantum information science research programs and establish SciDAC-like partnerships in underserved communities to develop new exascale-ready computational science environmental justice-related applications and simulations.
  - **ACCELERATE (+5M)** - **ASCR** will support the development of new AI/ML and data analysis algorithms and visualization tools to accelerate the design and deployment of clean energy technologies and promote energy-efficient computing.

FY 2023 ASCR Facilities

- The ASCR Facilities continue optimal operations in FY 2023.
- The **ALCF-3 Project** will continue acceptance testing while supporting exascale application testing and deployment.
- ESnet will continue to deploy upgraded real-time performance monitoring capabilities including host network flow, device performance, optical line, perfSONAR and ESnet6 high-touch packet telemetry data.
- The **ESnet6 Project,** completed in FY2022, will transition to operations.
- The **NERSC-9 Project** will complete with the acceptance of Phase 2 of Perlmutter in early FY2023 while continuing to plan for NERSC-10.
- In FY2023, the **OLCF** will complete the OLCF-5 project; support the final testing and deployment of the Exascale Computing Project's applications and software; and begin to transition to full operations.
- Planning will continue for working toward Critical Decision 1 for the **High Performance Data Facility** with a focus on incorporating information gathered in the Architecture Blueprint Activity.
- The ASCR Facilities Division, in partnership with the Research program, will initiate a subset of activities outlined in the **SC Integrated Research Infrastructure Architecture Blueprint Activity,** developed in FY 2022.

What's Next for ASCR Facilities Vendor Request for Information (RFI) Plans

- **Agency Priority Goal:** Sustain U.S. leadership in Advanced Computing technologies and enable continued progress in science and engineering applications
  - Engage community to identify science and engineering application needs
  - Engage vendors to identify new technologies that require Federal investment to meet the needs of mission critical science and engineering applications
  - Develop and implement Advanced Computing Technology Development and Deployment Strategy
- **Action for 3rd Quarter FY2022:** DOE Laboratories will be issuing a joint RFI to computing technology vendors to solicit input on their capabilities to to meet DOE requirements for future systems
- Over 35 companies are being targeted for preliminary briefings
  - HPC technologies for simulation, data analysis and AI
  - AI accelerators and systems, QC accelerators and systems, Cloud Architectures
  - Edge systems for data analysis and inference,
  - Advanced communications and data storage
  - Systems integration capabilities
- NDA briefings will feed into formal RFI (target early summer 2022)
- RFI responses will drive DOE and Laboratory planning for facilities strategy and roadmaps and potential investment in technology R&D (fall 2022)
- RFI process is a joint activity between DOE SC and NNSA ASC

Some other Highlights

Recognition of Our Community Members

2022 Class of National Academy of Engineering

Karen E. Wilcox, UT Austin

AEOLUS (MMICCs) Co-Director

2022 Class of National Academy of Engineering

George Em Karniadakis, Brown University

PhILMs MMICCS

2022 SIAM Activity Group on Supercomputing (SIAG/SC) Career Prize

Rob Falgout, LLNL

FASTMath (SciDAC) PI

SIAM President-Elect

Sven Leyffer, ANL

FASTMath (SciDAC) & Applied Math PI

Barney Maccabe retires from Oak Ridge National Laboratory

- Fostered collaborations among the DOE laboratories in the ASCR space
- Reorganized Computer Science and Mathematics Research at ORNL to better represent ASCR Priority Research Directions
- Active organizer for numerous workshops including SOS, ADAC, Smoky Mountains, and AI for Science
- Led the SNS data initiative and created the application engineering and software engineering research groups
- Next: Director of the Institute for the Future of Data and Computing, University of Arizona

Karen Devine Retires from Sandia National Laboratory

Karen made foundational contributions to HPC as part of the development team for the Zoltan and Trilinos scientific computing packages.

- Long time ASCR PI; SciDAC FASTMath Deputy Director
- 2019 Society of Women Engineers, Prism Award
- 2018, chair of the Activity Group on Computational Science and Engineering (SIAG/CSE) of SIAM
- 1999, Distinguished Young Alumni Award, Wilkes University

QSCOUT Testbed Spotlight on Progress
Winner of 2021 R&D100 Award

Achievement in QIS S&T Innovation Chain

The Quantum Scientific Computing Open User Testbed won an R&D100 award in the category of IT/Electrical.

Significance and Impact

This award recognizes the unique benefits of QSCOUT as accessible quantum hardware

Details

- The application emphasized how the low-level access afforded by QSCOUT – which is not available in commercial quantum systems – enables researchers to study the behavior of quantum hardware. This type of study is necessary to learn the best way to build a bigger quantum machine relevant to solving problems of interest to the DOE.
- Established in 1963, the R&D 100 Awards is the only science and technology awards competition that recognizes new commercial products, technologies and materials for their technological significance. Only 100 winners are announced each year and are selected by an expert panel of judges.

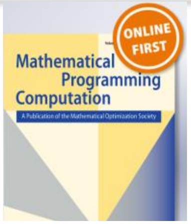
https://www.rdworldonline.com/2021-rd-100-award-winners-announced-in-analytical-test-and-it-electrical-categories/

- An international, community-driven event to promote quantum science to the general public
- Like Exascale Day, Pi Day, Mole Day, Nano Day
- Date chosen for Planck’s constant, 4.14 x 10^{-15} eV·s
- Federal agencies coordinating for greater impact
  - Social media posts using #WorldQuantumDay
  - 30-second selfie videos from quantum scientists
  - Images of federally-funded quantum research on quantum.gov
  - Factsheets on Planck’s constant and the National Quantum Initiative

Some ASCAC Agenda Details

- NATIONAL QIS RESEARCH CENTERS – *Irfan Siddiqi, Lawrence Berkeley National Laboratory*
- COMMUNITY OF INTEREST UNCONFERENCE – *Ian Foster, Argonne National Laboratory and Amber Boehnlein, Jefferson National Accelerator Laboratory*
- EXASCALE UPDATE – *Doug Kothe, Oak Ridge National Laboratory and Lori Diachin, Lawrence Livermore National Laboratory*
- POLARIS: A SCALABLE TESTBED TOWARDS AURORA, *Ti Leggett, Argonne National Laboratory*
- REPORT FROM COV – *Alexandra Landsberg, ASCAC*
- UPDATE FROM THE WORKING GROUP ON COLLABORATION WITH NNSA AND NCI – *Tony Hey, ASCAC*
- UPDATE ON FRONTIER EXASCALE SYSTEM AND EARLY SCIENCE*, Al Geist, Oak Ridge National Laboratory*
- UPDATES ON SOFTWARE STEWARDSHIP RFI AND COMPUTER SCIENCE WORKSHOPS– *Hal Finkel ASCR*
- QUANTUM REQUEST FOR INFORMATION - *Ceren Susut, ASCR*

Two 2021 Best Papers in Flagship Journals



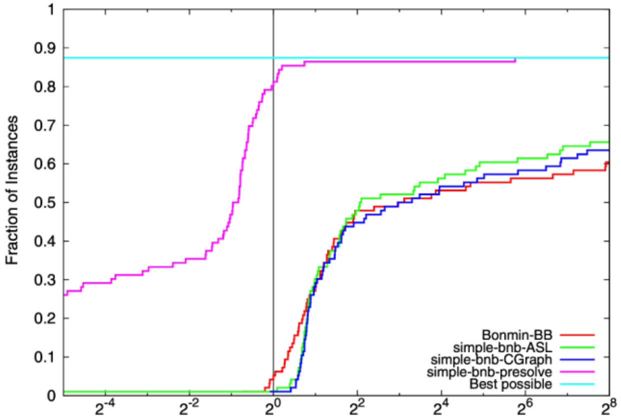
ASCR Math Base and SciDAC

Two Best Paper Awards for Optimization Research

1. **Mathematical Programming C Best Paper Prize for Minotaur, an open-source framework for mixed-integer nonlinear optimization.**
2. **INFORMS Simulation Society Outstanding Simulation Publication Award for research in convergence rate of stochastic trust-region (TR) methods.**

Significance and Impact

DOE optimal design applications: (1) Minotaur for power-grid expansion, and (2) stochastic TR methods for quantum algorithms.



Performance profile showing impact of presolve and syntax-tree reformulation unique to MINOTAUR.

Research Details

- Minotaur exploits problem structure, to solve larger problems orders of magnitude faster, and a modular approach making it easily extensible.
- Convergence rate analysis demonstrates superior iteration complexity of variance-adaptive stochastic TR methods over stochastic gradient methods.

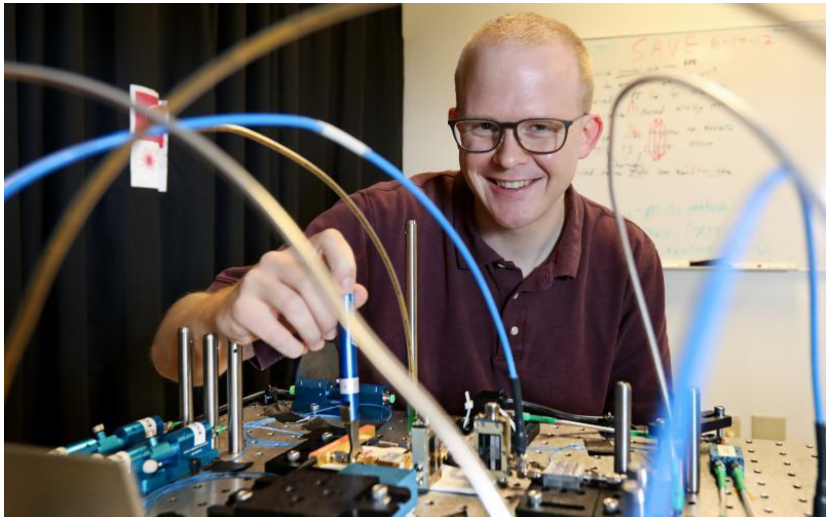
- Ashutosh Mahajan, Sven Leyffer, Jeff Linderoth, James Luedtke, and Todd Munson. Minotaur: A Mixed-Integer Nonlinear Optimization Toolkit. *Mathematical Programming Computation*, November 2020. DOI:10.1007/s12532-020-00196-1
- Jose Blanchet, Coralia Cartis, Matt Menickelly, and Katya Scheinberg. “Convergence Rate Analysis of a Stochastic Trust-Region Method via Supermartingales,” *INFORMS Journal on Optimization*, 1(2), 2019. DOI:10.1287/ijoo.2019.0016

ANL: Sven Leyffer, Matt Menickelly, and Todd Munson.

Giant leap toward quantum internet realized with Bell state analyzer

The Science
A multi-institutional team featuring ORNL's Joe Lukens has made strides toward a fully quantum internet by designing and demonstrating the first ever Bell state analyzer for frequency bin coding. Measuring Bell states is critical to performing many of the protocols necessary to perform quantum communication and distribute entanglement across a quantum network. The team's method represents the first Bell state analyzer developed specifically for frequency bin coding, a quantum communications method that harnesses single photons residing in two different frequencies simultaneously.

The Impact
The analyzer was designed with simulations and has experimentally demonstrated 98% fidelity for distinguishing between two distinct frequency bin Bell states. This incredible accuracy should enable new fundamental communication protocols necessary for frequency bins.



ORNL's Joseph Lukens runs experiments in an optics lab. Credit: Jason Richards/ORNL, U.S. Dept. of Energy

PI(s)/Facility Lead(s): Joe Lukens (ORNL)
ASCR Program/Facility: N/A
ASCR PM: Lali Chatterjee
Funding: Office of Science through the Early Career Research Program
Publication for this work: Navin B. Lingaraju, Hsuan-Hao Lu, Daniel E. Leaird, Steven Estrella, Joseph M. Lukens, and Andrew M. Weiner. "Bell state analyzer for spectrally distinct photons," Optica Vol. 9, Issue 3, pp. 280-283 (2022).

APPFL: The Argonne Privacy-Preserving Federated Learning Framework

Scientific Achievement

Privacy-preserving federated learning framework APPFL enables supervised learning of a model on distributed sensitive datasets while preserving the data privacy

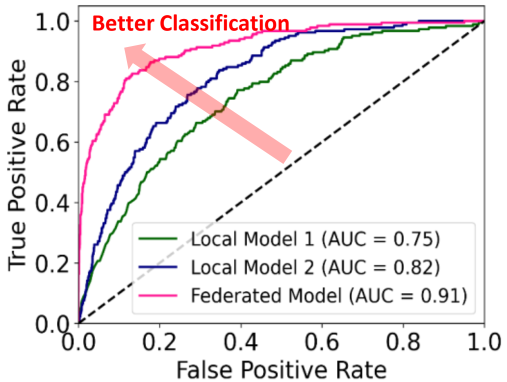
Significance and Impact

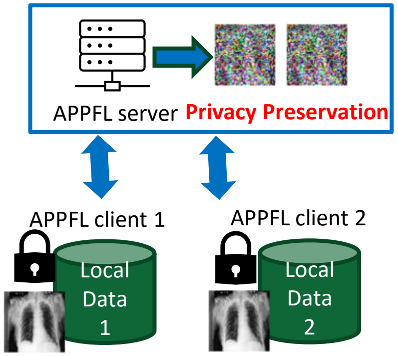
APPFL will enable research collaborations across countries and institutions while addressing the privacy and data shift challenges in many DOE applications (e.g., scientific machine learning, critical infrastructure)

Research Details

- Novel distributed optimization algorithms with differential privacy result in better convergence and learning performance
- In collaboration with medical institutions, APPFL is used to train image classification models on private chest x-ray data
- APPFL used for federated control of power system operations maintaining data privacy against an adversary

Privacy Preservation: *With stronger privacy, APPFL can prevent reconstruction of chest X-ray images from model weights by leveraging the gradient transfer during federated learning*





Data Shift Challenge: *Federated learning produces more accurate models in classifying chest X-ray image for COVID-19 compared to the models trained on local datasets*

Ryu, Kim, Kim, Madduri. “APPFL: Open-Source Software Framework for Privacy-Preserving Federated Learning” *2022 IEEE IPDPS Workshop (accepted)*; https://github.com/APPFL/APPFL

Ryu, Kim. “Differentially Private Federated Learning via Inexact ADMM with Multiple Local Updates” *arXiv:2022.09409*, 2022

Ryu, Kim. “A Privacy-Preserving Distributed Control of Optimal Power Flow” *IEEE Transactions on Power Systems*, 2021

ASCR Applied Math PIs: Kibaek Kim and Ravi Madduri

Design of Many-Core Big Little µBrains for Energy-Efficient Embedded Neuromorphic Computing

The Science

- Massive improvements in the energy efficiency of artificial intelligence are needed to sustain continued advancement and enable new applications.
- Specialized hardware for spiking neural networks promise significant improvements in energy efficiency.
- State-of-the-art digital designs use crossbar-connected cores, but a significant fraction of the resources in each crossbar remains underutilized.
- The on-chip network becomes the primary energy and performance bottleneck as these systems scale up.
- A new approach, using hardware-software co-design, combining ***µ***Brain cores using a novel segmented bus (SB) interconnect and system software called SentryOS (compared to Intel's Loihi):
    - Reduces energy between 37% and 98%
    - Reduces latency between 9% and 25%
    - Increases throughput between 20% and 36%

Anup Das, DOE/ASCR Early-Career Awardee, 2021.

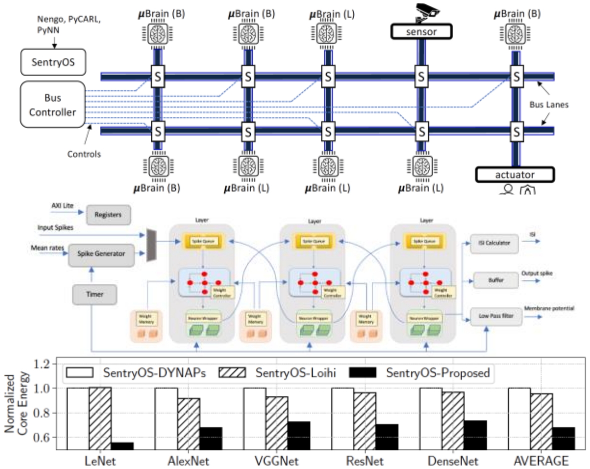


*Fig: (a) Design of a many-core neuromorphic hardware with big-little **µ**Brain cores and segmented bus (SB) interconnect. (b) A µBrain design implemented on FPGA. (c) µBrain-based many-core hardware with SB is better than DYNAPs and Intel's Loihi.*

The Impact

- The new approach features better scaling than previous digital neuromorphic designs, promising to enable large-scale applications.
- The segmented bus (SB) interconnect can enable virtualization of neuromorphic systems, enabling hardware sharable by many users.
- SentryOS can be used for faster application development and deployment on neuromorphic hardware.

PI(s)/Facility Lead(s): Anup Das
Collaborating Institutions: Drexel University, Imec (Netherlands and Belgium)
ASCR Program/PM: ECRP / Hal Finkel
Publication(s) for this work: L. M. Varshika, et al., "Design Of Many-core Big Little µBrains For Energy-efficient Embedded Neuromorphic Computing," *Design Automation and Test in Europe (DATE) Conference* (2022).

Distributed, Intelligent, and Scalable COmputing DISC Lab

Precision tomography of a three-qubit electron-nuclear quantum processor in silicon

Scientific Achievement

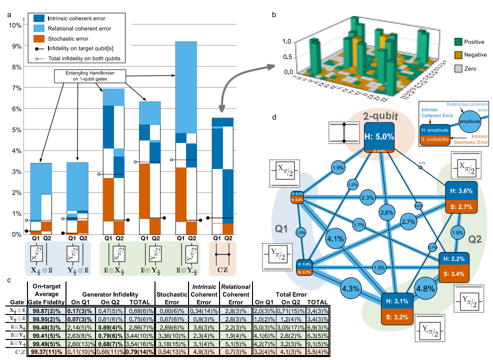
We used a customized and streamlined form of gate set tomography to achieve the most precise, detailed characterization ever of two qubits. This analysis identified unexpected, performance-limiting errors in the quantum gates, and assisted the experimentalists in identifying the source.

Significance and Impact

This collaboration with UNSW established that donor spins in silicon are a viable quantum computing architecture. The new GST analysis method provides unprecedented insights into the errors experienced by quantum gates and represents a gold standard for characterization of qubit dynamics.

Research Details

We introduced reduced error generator models that can distinguish between statistically significant and statistically insignificant errors. We built new metrics of gate error based on the error generators, and a new gauge-invariant representation of errors. These techniques enabled a simple, complete and intuitive picture of gate errors.



"Precision tomography of a three-qubit electron-nuclear quantum processor in silicon", Mądzik, Asaad, Youssry, Joecker, **Rudinger, Nielsen, Young, Proctor**, **Baczewski**, Laucht, Schmitt, Hudson, Itoh, Jakob, Johnson, Jamieson, Dzurak, Ferrie, **Blume-Kohout**, Morello
***Nature* 601, 348–353 (2022) (Cover)**

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U.S. DEPARTMENT OF ENERGY Office of Science

Engineering high-coherence superconducting qubits


QUBITS

REVIEWS

Check for updates

Engineering high-coherence superconducting qubits

Irfan Siddiqi[1,2]

NATURE REVIEWS | MATERIALS VOLUME 6 | OCTOBER 2021 | 875

Noise source	Mitigation strategy
Two-level system (TLS) defects	Etching and passivation to remove amorphous layers; use of crystalline dielectrics and ordered Josephson junction barriers. The underlying microscopic mechanisms need to be identified
Quasiparticles and phonons	Normal metal/low-gap superconducting traps to remove quasiparticles from the qubit area; acoustic absorbers and frequency-tailored structures to suppress phonon propagation and secondary pair breaking
$1/f$ magnetic flux noise	Initial work indicates noise reduction with capping layers. Need to identify precisely the microscopic origin to develop robust, tailored elimination strategies

Review article as published in Nature Reviews Materials. Primary sources of noise in superconducting qubits and mitigation approaches.

Scientific Achievement

Review article on materials imperfections and sources of noise impacting coherence maximization in superconducting circuits.

Significance and Impact

Details the continuum of tradeoffs to achieve a given performance level, from simple circuits with perfected materials to complex circuits that can accommodate noisy materials.

Research Details

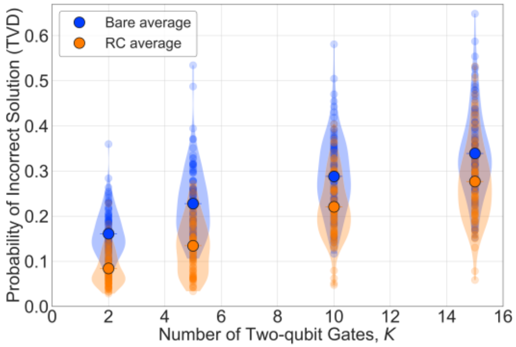
- Surfaces, interfaces, and quasiparticles play key roles in limiting device coherence.
- Circuit elements capable of accessing different qubits are required to advance quantum computing.
- Achieving quantum computational advantage will ultimately require a full-scale redesign of the materials and wiring layers in a processor, targeting the high-fidelity generation, preservation, and control of many-body entanglement.

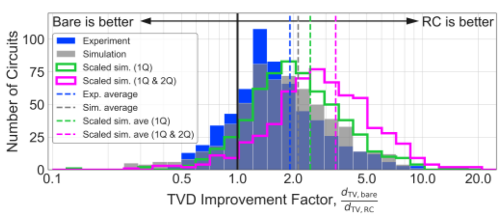
I. Siddiqi, www.nature.com/articles/s41578-021-00370-4, *Nature Reviews Materials volume 6, pages 875–891 (2021).*

Work was performed at Lawrence Berkeley National Laboratory

BERKELEY LAB

Scalable Quantum Computing via Randomized Compiling





Upper: RC improves the performance of random circuits at all circuit depths tested. Performance is quantified by the Total Variation Distance (TVD) = the probability of measuring an incorrect solution.

Lower: Most circuits are improved under RC for the quantum Fourier transform. Simulations using measured error rates show good agreement. RC performance will improve as error rates decrease.

Scientific Achievement

Demonstrated a randomized compiling (RC) protocol to suppress coherent errors and increase quantum algorithm fidelity.

Significance and Impact

RC mitigates coherent errors in quantum circuits, resulting in higher accuracy of the quantum computational output; this method also enables accurate predictions of algorithm performance from measured qubit error rates.

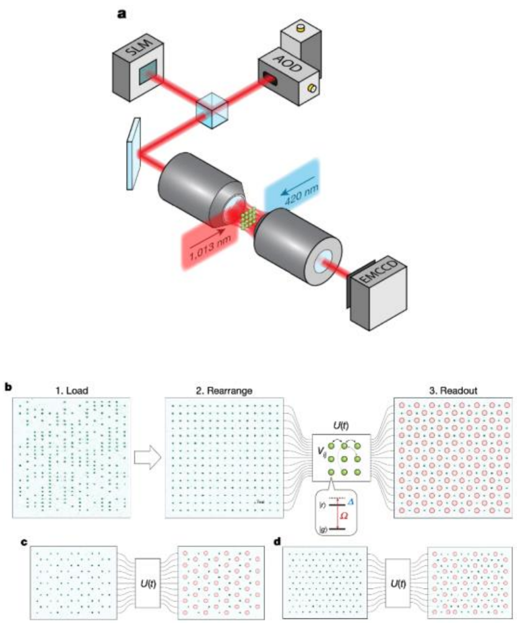
Research Details

- Coherent errors accumulate more quickly than stochastic errors during algorithm execution, and are a leading factor that limit algorithm performance.
- RC converts coherent errors into stochastic noise by combining the output of many randomized quantum circuits that are logically equivalent.
- Experimentally, we show performance gains under RC for the quantum Fourier transform algorithm and random circuits.
- Algorithm performance was predicted independently, using experimentally-measured error rates.

A. Hashim et al., *Phys. Rev. X 11, 041039* (2021)

Work was performed at the Lawrence Berkeley National Laboratory

Quantum phases of matter on a 256-atom programmable quantum simulator



a) The experimental platform with a 2D array of optical tweezer traps. b-d) The sequence of loading and rearranging atoms to simulate a two-dimensional spin model.

S. Ebadi, et. al., *Nature* **595**, 227-232 (2021)

Accomplishment

Studied quantum phases of a spin system using a programmable quantum simulator based on a two-dimensional array of neutral atoms in Rydberg states.

Significance and Impact

Demonstrates a new tool for investigations of complex matter, including exotic quantum phases and non-equilibrium dynamics.

Details

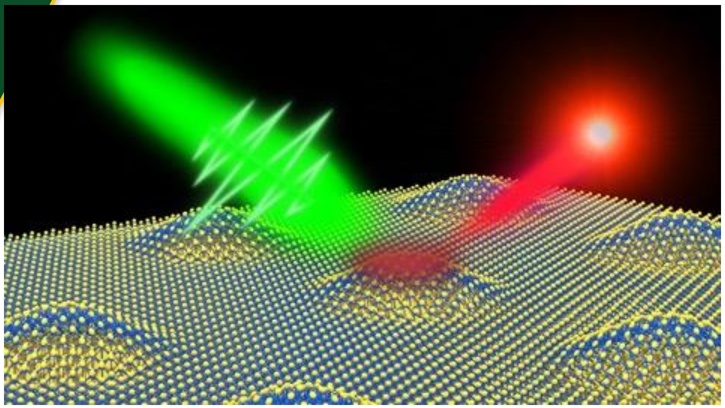
- Simulated quantum phases and phase transitions which had not been previously observed in a (2 + 1)-dimensional Ising spin model.
- Implemented the simulation on arrays of 64 to 256 neutral atoms with tunable interactions, using optical tweezer traps.
- Created a platform also suitable for quantum information processing and implementation of hardware-efficient quantum algorithms.

Work was performed at Harvard University, the University of Innsbruck, UC Berkeley, and MIT

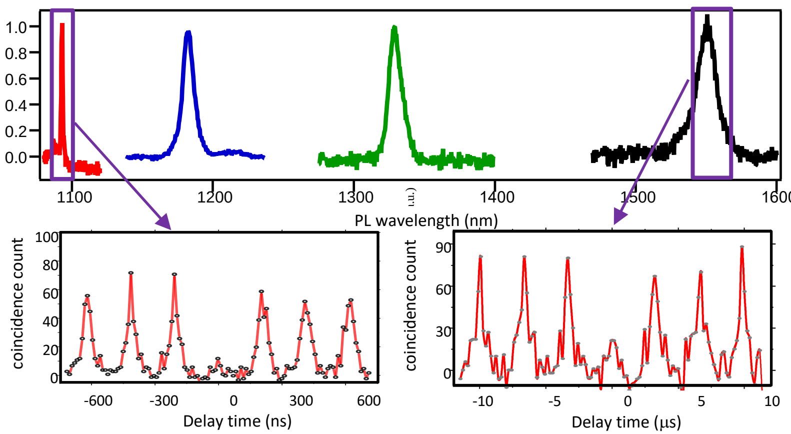
QUANTUM SYSTEMS ACCELERATOR
Catalyzing the Quantum Ecosystem

Telecom Quantum Emitters:

Strained Atomically Thin $MoTe_2$ as Deterministic Single Photon Sources



Atomically-thin $MoTe_2$ layer (blue and yellow lattice) on strain-inducing nanopillars as site-controlled telecom-wavelength quantum emitters for coupling to optical fibers with minimal loss. Single photons (red) is generated upon optical excitation (green)



PL spectra of 4 QEs covering 1100 to 1600 nm spectra range.

2nd order photon correlation spectra of QE emitting at 1100 nm (red) and 1550 nm (black).

Scientific Achievement

Site-controlled, bright quantum light emitters (QEs) capable of > 90% single photon purity at 1550 nm telecom band is achieved for the first time in two dimensional, mono- and multi-layer $MoTe_2$ via local strain engineering.

Significance and Impact

Enable integration of 2D material based quantum light sources into existing fiber-based optical communication networks for practical implementation of quantum cryptography, transduction and sensing applications.

Research Details

- QEs were created by straining mon- and muti-layered $MoTe_2$ on top of an array of nanopillars with ~ 150 nm diameter and ~ 100 nm height.
- Layer thickness of $MoTe_2$ can be varied from mono-layer to >10 layer to tune the emission wavelength of the QEs from 1100 to 1600 nm covering both O and C telecommunication bands.
- Quantum optic experiments revealed that single photon emission (SPE) with purity >90% can be achieved at 10 K and SPE survive up to 77 K.
- Our polarization resolved, magneto PL experiment revealed existence of anisotropically split fine structures states at zero field and valley polarization of QEs under 8T magnetic field.

Zhao, Huan, et al. "Site-Controlled Telecom-Wavelength Single-Photon Emitters in Atomically-thin MoTe2." *Nature Communications* 2021, DOI : 10.1038/s41467-021-27033-w