FOSSIL ENERGY WORKSHOP ON

QUANTUM INFORMATION SCIENCE & TECHNOLOGY

NOVEMBER 19–20, 2019

NATIONAL ENERGY TECHNOLOGY LABORATORY

PITTSBURGH, PA

U.S. DEPARTMENT OF ENERGY | Office of Fossil Energy | NETL NATIONAL ENERGY TECHNOLOGY LABORATORY

WORKSHOP CHARGE/SCOPE

Quantum Information Science (QIS) is expected to profoundly change the practice of science and engineering in the coming decades. It is a rapidly progressing field, fueled by large investments from the private sector and governments. Its importance to the U.S. economy and national security is underscored by the National Quantum Initiative Act passed in December 2018. QIS includes quantum sensing, quantum communications, quantum simulation experiments, and quantum computation. QIS Technology exploits quantum phenomena for performing tasks that are impossible to do today, such as finding prime factors of large numbers or elucidating reaction mechanisms in complex chemical systems.

The opportunities for applying QIS to problems encountered in fossil energy technology development are not known today. This workshop aims to bring together, for the first time, experts in these fields to exchange information and explore potential research opportunities for QIS to advance fossil energy. The goal of the workshop is to develop a set of priority research opportunities that can inform future research efforts in QIS and build a community of next-generation researchers at the intersection of QIS and fossil energy.

WORKSHOP ORGANIZING COMMITTEE

Madhava Syamlal (Chair)
Jeremy Levy (Co-chair)
Regis Conrad
Yuhua Duan
Coriana Fitz
Christopher Matranga
Darren Mollot
Michael Nowak
Paul Ohodnicki
Hari Paudel
Massood Ramezan
Jennifer Stein
Ke Xu

NATIONAL ENERGY TECHNOLOGY LABORATORY
www.netl.doe.gov

<P|Q|I> PITTSBURGH QUANTUM INSTITUTE
www.pqi.org

AGENDA

TUESDAY, NOVEMBER 19, 2019

8:00 – 8:30 A.M. — CHECK-IN/BREAKFAST

8:30 – 9:00 A.M. — WELCOME/INTRODUCTION
Randall W. Gentry (NETL) on behalf of Brian J. Anderson (NETL)
Madhava (Syam) Syamlal (NETL)
Jeremy Levy (U. of Pittsburgh/PQI)

9:00 – 9:30 A.M. — DOE PROGRAM IN QUANTUM INFORMATION SCIENCE
Barbara Helland (U.S. Department of Energy)

9:30 – 10:00 A.M. — KEYNOTE, FOSSIL ENERGY
Charles McConnell (U. of Houston)

10:00 – 10:15 A.M. — BREAK

10:15 – 10:45 A.M. — KEYNOTE, QUANTUM INFORMATION SCIENCE
Celia Merzbacher (Quantum Economic Development Consortium)

10:45 – 12:15 P.M. — PANEL 1 – QUANTUM SENSORS/DETECTORS AND QUANTUM EXPERIMENTS
Panel Moderator: Randall W. Gentry (NETL)
Panel Members: Chethan Acharya (Southern Company), Henry Du (Stevens Institute of Technology), Carl Williams (NIST), Benjamin Lawrie (ORNL), Michael Hatridge (U. of Pittsburgh), Benjamin Gilbert (LBNL), Supratik Guha (ANL)

12:15 – 1:15 P.M. — LUNCH

1:15 – 2:45 P.M. — PANEL 2 – QUANTUM COMPUTATION FOR MACHINE LEARNING, AI, AND OPTIMIZATION
Panel Moderator: David Miller (NETL)
Panel Members: Zlatko Minev (IBM), Nick Sahinidis (Carnegie Mellon), Earl Scime (WVU), Aaron Hussey (Integral Analytics), John Siirola (SNL), Michael Flatté (U. of Iowa)

2:45 – 3:00 P.M. — BREAK

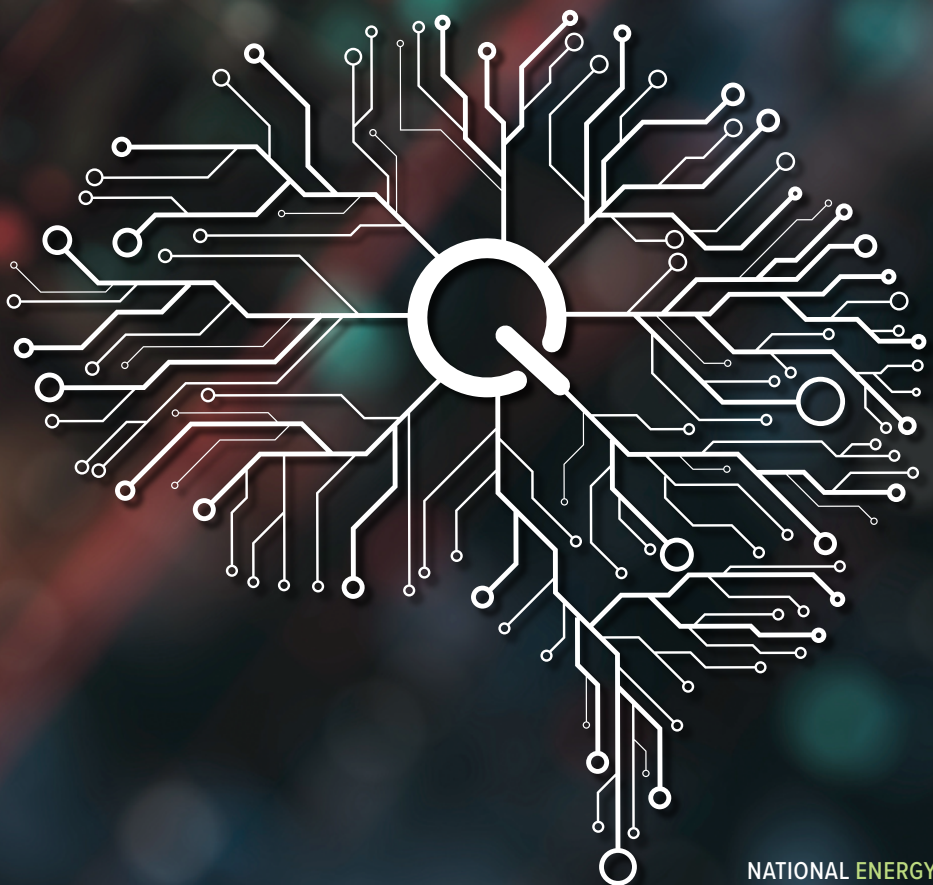
3:00 – 4:30 P.M. — PANEL 3 – QUANTUM COMPUTATION/SIMULATION FOR CHEMISTRY AND MATERIALS
Panel Moderator: Jeremy Levy (U. of Pittsburgh/PQI)
Panel Members: Philip Richerme (Indiana U.), Götz Veser (U. of Pittsburgh), Ignasi Palou-Rivera (RAPID Manufacturing Institute), Raphael Pooser (ORNL), Mike Santos (U. of Oklahoma), Andrew Baczewski (SNL)

4:30 P.M. — ADJOURN

AGENDA

WEDNESDAY, NOVEMBER 20, 2019

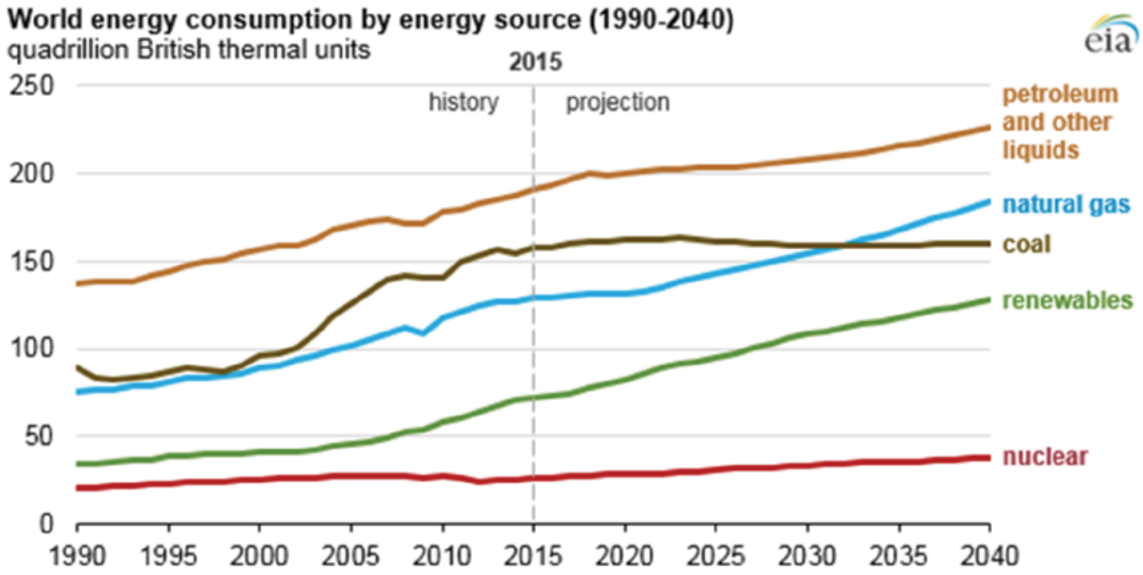
8:00 – 8:30 A.M.	CHECK-IN/BREAKFAST
8:30 – 10:00 A.M.	PANEL 4 – QUANTUM COMPUTATION FOR PROCESS MODELING/CFD AND QUANTUM NETWORKING Panel Moderator: Richard Bajura (WVU) Panel Members: Peyman Givi (U. of Pittsburgh), Michael Leuenberger (U. of Central Florida), Stephen Bush (GE), Randy Smith (SNL)
10:00 – 10:15 A.M.	BREAK
10:15 – 12:15 P.M.	FACILITATED BRAINSTORMING SESSION – OPPORTUNITIES FOR FOSSIL ENERGY APPLICATIONS
12:15 – 12:30 P.M.	CLOSING REMARKS
12:30 – 1:30 P.M.	LUNCH
1:30 P.M.	ADJOURN



FOSSIL ENERGY

Fossil Energy Will Remain the Foundation for World Energy Demand for Decades to Come

Fossil energy provides quality of life to millions of Americans, sustains America's manufacturing and high-technology industries, fuels economic growth, and stimulates technical innovation. Tremendous technological effort and innovation has diversified the energy portfolio to meet ever increasing global demand. Even so, studies project that fossil energy will be required to supply expanding world energy markets and will continue to satisfy nearly 80 percent of energy demand for decades.



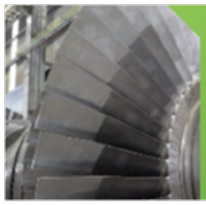
Advanced Technologies Are Critical to the Future of Fossil Energy

Advanced technologies enable fossil fuels to produce the clean, reliable, and affordable energy needed to increase domestic manufacturing, invest in improving our Nation's energy infrastructure, improve electrical grid reliability and resilience, expand domestic energy production, educate America's future scientists and engineers, revitalize the workforce, and support U.S. energy and national security goals.

Fossil Energy Research Priorities

Six bold fossil energy research and development priorities have the potential to advance the Nation's entire energy system.

- Develop the coal plants of the future by advancing small-scale modular coal plants of the future, which are highly efficient and flexible with near-zero emissions
- Modernize the existing coal fleet by improving the performance, reliability, and efficiency of the existing coal-fired fleet
- Reduce the cost and risk of carbon capture, utilization, and storage (CCUS) to enable wider deployment
- Advance big data by optimizing recovery of oil and gas resources with real-time analysis and machine learning
- Address the energy water nexus by improving efficient use of water resources
- Develop rare earth elements separation and recovery technologies and processes to manufacture valuable products from coal to address current global market and process economics



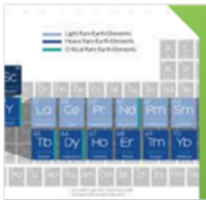
Develop the Coal Plants of the Future

Expand the Use of Big Data by Leveraging Artificial Intelligence

Modernize the Existing Coal Fleet

Energy Water Nexus

Reduce the Cost of CCUS



Rare Earth Elements / Critical Materials / Coal Products

These research priorities are currently supported through the following initiatives:

- Advancing the design of structural and functional materials
- Leveraging simulation-based engineering with “hands-on” chemical engineering capabilities that closely integrate laboratory experiments with computational methodologies
- Predicting physical, chemical, and biological characteristics of extreme environments through wide time and length scales
- Applying machine learning-based estimation tools to enable comprehensive evaluation of complex and diversified energy systems

Quantum Information Science (QIS) and Fossil Energy Technology Development

The opportunities for applying Quantum Information Science (QIS) to problems encountered in fossil energy technology development are not known today. However, experts in these fields are exchanging information and exploring potential research opportunities for QIS to advance fossil energy. The goal is to develop a set of priority research opportunities that can inform future research efforts in QIS and build a community of next-generation researchers at the intersection of QIS and fossil energy.

Promising areas include:

- Geomaterials Sensing; Geophysical Surveying
- Materials Discovery/Combinatorial Optimization
- Materials Properties: Stress and Fatigue Analysis
- Process Simulation Including CFD
- Infrastructure Monitoring and Cybersecurity
- AI/Machine Learning

QUANTUM INFORMATION SCIENCE

Quantum Information Science is expected to profoundly change the practice of science and engineering in the coming decades

Quantum Information Science (QIS) uses distinct behaviors of quantum systems and is expected to lay the foundation for the next generation of computing and information processing, as well as an array of other innovative technologies in sensing and related applications. QIS comprises four distinct areas:

Quantum Sensing[1]

Exploits the strong sensitivity of quantum systems to external disturbances to measure physical quantities such as magnetic or electric fields. Potential applications include[2]

- Atomic Clocks
- Radiation and Gas Measurement
- Medical Imaging

Quantum Networking

Transmits information with the help of "entangled" particles – whose quantum state cannot be described independently, even when they are separated by a large distance.

- Argonne National Laboratory, Fermilab, and University of Chicago are partnering to "teleport" information across a 30-mile distance between the two labs.

Quantum Simulation[3]

Involves using a "controllable quantum system to study another less controllable or accessible quantum system."

- Could be implemented with analog devices that would be easier to construct than quantum computers. Potential applications include[4]
  - Materials Science
  - Catalysis
  - Molecular Systems

Quantum Computing[5]

Quantum computers use quantum bits, or qubits, which represent the values 0 or 1, or some combination of both at the same time (known as a "superposition"). Intrinsically interconnected ("entangled") qubits can access an exponentially larger parameter space compared with classical bits, enabling quantum computers to solve problems impossible on classical computers. Potential applications include[6]

- Encryption and Cybersecurity
- Financial Services
- Drug Research and Development
- Supply Chain Logistics
- Faster Data Analysis (Big Data)

1 Degen CL, Reinhard F, Cappellaro P. Quantum Sensing. DOI: 10.1103/RevModPhys.89.035002. 2017
2 Jonathan O'callaghan, "Quantum technology could revolutionise the detection and treatment of diseases." Horizon Magazine, Horizon: The EU Research & Innovation Magazine, June 24, 2019 *https://horizon-magazine.eu/article/how-quantum-technology-could-revolutionise-detection-and-treatment-diseases.html*
3 Georgescu IM, Ashhab S, Nori F. Quantum Simulation. arXiv:1308.6253v3. 2014
4 Nicole Hemsoth, "Intel's Quantum Efforts Tied to Next-Gen Materials Applications" The Next Platform, Jan. 9, 2019 *https://www.nextplatform.com/2019/01/09/intels-quantum-efforts-tied-to-next-gen-materials-applications/*
5 National Academies of Sciences, Engineering, and Medicine. 2018. Quantum Computing: Progress and Prospects. The National Academies Press, Washington, DC. DOI: *https://doi.org/10.17226/25196*.
6 John Loeffler "Five Intractable Problems Quantum Computing Will Solve" Interesting Engineering, Dec 15, 2018 *https://interestingengineering.com/5-intractable-problems-quantum-computing-will-solve*

QUANTUM INFORMATION SCIENCE

National Quantum Initiative Act

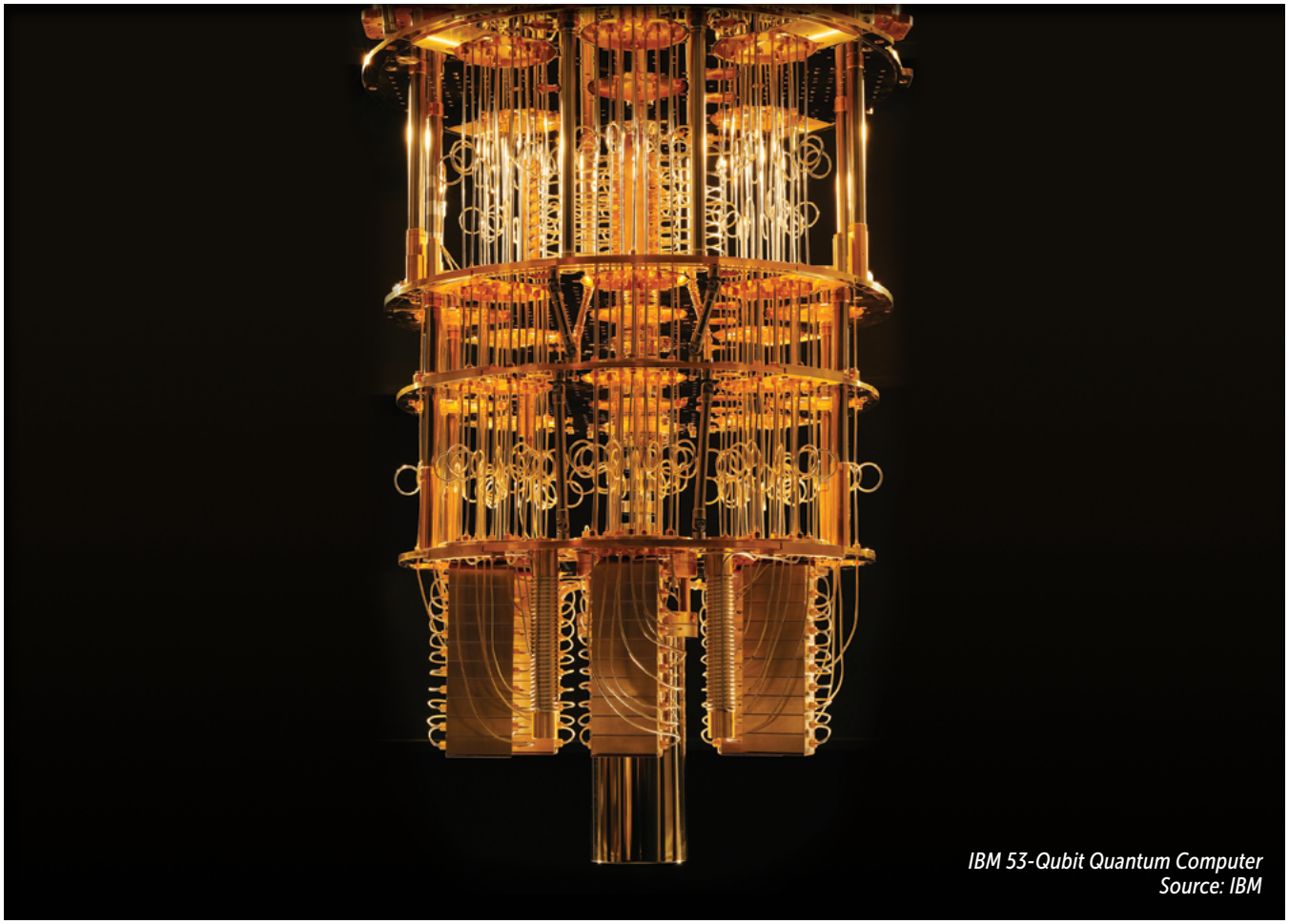
Signed into law on 21 December 2018, creating a multiagency program spanning the National Institute of Standards and Technology, National Science Foundation, and Department of Energy.

FY20 budget request

- NIST – $40 million to build out Quantum Economic Development Consortium and expand quantum research institutes at the University of Maryland and the University of Colorado, Boulder[7]
- NSF – $106 million to support Quantum Leap Challenge Institutes[8]
- DOE – $168 million; the act directs DOE to establish 2 to 5 "National Quantum Information Science Research Centers"[9]

Prospects for Enterprise Quantum Computing

- Among Gartner Top 10 Strategic Technology Trends for 2019[10]
- By 2023, 20% of organizations will be budgeting for quantum computing projects[11]
- Annual budget for enterprise quantum computing reported to rise from $39.2 million in 2017 to $2.2 billion by 2025[12]



IBM 53-Qubit Quantum Computer
Source: IBM

7 https://www.aip.org/fyi/2019/fy20-budget-request-national-institute-standards-and-technology
8 https://www.aip.org/fyi/2019/fy20-budget-request-national-science-foundation
9 https://www.aip.org/fyi/2019/fy20-budget-request-doe-office-science
10 https://www.gartner.com/smarterwithgartner/gartner-top-10-strategic-technology-trends-for-2019/
11 https://www.gartner.com/smarterwithgartner/the-cios-guide-to-quantum-computing/
12 https://www.tractica.com/newsroom/press-releases/enterprise-quantum-computing-market-to-reach-2-2-billion-by-2025/

BIOS: WELCOME/INTRODUCTION

WELCOME/INTRODUCTION

Brian J. Anderson, Ph.D. | National Energy Technology Laboratory

Director

Dr. Brian J. Anderson is director of the U.S. Department of Energy's (DOE) National Energy Technology Laboratory (NETL). Anderson manages the complete NETL complex, including delivery and execution of the Laboratory's mission, and national programs in fossil energy. Anderson came to NETL from West Virginia University (WVU) where he served as the director of the WVU Energy Institute. He has a long history of collaboration with NETL and other DOE national laboratories. He served NETL as the coordinator of the International Methane Hydrate Reservoir Simulator Code Comparison study and in 2011 was awarded a Secretary Honor Achievement Award from the Secretary of the Department of Energy for his role on the Flow Rate Technical Group, a team spanning multiple national laboratories that worked in response to the Deepwater Horizon oil spill.

Dr. Anderson is also a recipient of the 2012 Presidential Early Career Award for Scientists and Engineers, the highest honor bestowed by the U.S. government on science and engineering professionals in the initial stages of their careers. He served as a member of the National Academies of Sciences, Engineering, and Medicine (NASEM) Roundtable on Unconventional Hydrocarbon Development. Anderson earned his bachelor's degree in chemical engineering in 2000 at WVU and his master's and doctorate in chemical engineering from the Massachusetts Institute of Technology (MIT) in 2004 and 2005 respectively. Anderson's research interests include molecular, reservoir, and multiscale modeling and simulation applied to energy and biomedical systems.

Madhava (Syam) Syamlal, Ph.D. | National Energy Technology Laboratory

Senior Fellow for Computational Engineering

Dr. Madhava Symlal oversees the development of computational science and engineering capabilities for applications to energy technology development. Also, he is DOE Technical Director of University Coalition for Fossil Energy Research and leads an effort under DOE's Exascale Computing Project. He holds degrees in chemical engineering: B.Tech from IIT (BHU), India and MS and PhD from IIT, Chicago. His research is in multiphase computational fluid dynamics (CFD); he has made numerous contributions to the theory and numerics and the open-source code MFIX. He led an effort to develop Aspen Plus® and FLUENT® co-simulations and served as the founding Technical Director of Carbon Capture Simulation Initiative (CCSI), which developed tools for modeling carbon capture devices and processes. He is a fellow of American Institute of Chemical Engineers (AIChE) and the recipient of numerous awards, including R&D100 awards, DOE Secretary's Achievement Honor Award, and AIChE's Fluidization Process Recognition Award.

Jeremy Levy, Ph.D. | University of Pittsburgh/PQI

Distinguished Professor of Condensed Matter Physics

Dr. Jeremy Levy is a Distinguished Professor of Condensed Matter Physics at the University of Pittsburgh in the Department of Physics and Astronomy, and Director of the Pittsburgh Quantum Institute. He received an A.B. degree in physics from Harvard University in 1988, and a Ph.D. degree in physics from UC Santa Barbara in 1993. After a postdoctoral position at UC Santa Barbara, he joined the University of Pittsburgh in 1996. His research interests center around the emerging field of oxide nanoelectronics, experimental and theoretical realizations for quantum computation, semiconductor and oxide spintronics, quantum transport and nanoscale optics, and dynamical phenomena in oxide materials and films.

Dr. Levy is Director of the Pittsburgh Quantum Institute, the Center for Oxide-Semiconductor Materials for Quantum Computation, a Multidisciplinary University Research Initiative (MURI) on Quantum Preservation, Simulation and Transfer in Oxide Nanostructures, and a NSF Nanoelectronics for 2020 and Beyond program, and is a Class of 2015 National Security Science and Engineering Faculty Fellow (NSSEFF). He is a Fellow of the American Physical Society, and is the recipient of the 2008 Nano50 Innovator Award, and the NSF Career Award. He has received the University of Pittsburgh's Chancellor's Distinguished awards for research (2004, 2011) and teaching (2007).

BIOS: KEYNOTE TALKS

DOE PROGRAM IN QUANTUM INFORMATION SCIENCE

Barbara Helland | U.S. Department of Energy

Associate Director of the Office of Science's Advanced Scientific Computing Research (ASCR)

Barbara Helland is currently the Associate Director of the Office of Science's Advanced Scientific Computing Research (ASCR) program. In addition to her Associate Director duties, she is leading the development of the Department's Exascale Computing Initiative to deliver a capable Exascale system by 2021. Ms. Helland previously served as ASCR's Facilities Division Director. Prior to assuming the role of Division Director, she served as the Program Manager for ASCR's Argonne and Oak Ridge Leadership Computing Facilities and the National Energy Research Scientific Computing Center. She was also responsible for the opening ASCR's facilities to national researchers, including those in industry, through the expansion of the Department's Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program. Prior to DOE, Ms. Helland developed and managed computational science educational programs at Krell Institute. She also spent 25 years at Ames Laboratory working closely with nuclear physicists and physical chemists to develop real time operating systems and software tools to automate experimental data collection and analysis and in the deployment and management of lab-wide computational resources. She received B.S. in Computer Science and a M. Ed in Organizational Learning and Human Resource Development from Iowa State University.

KEYNOTE, FOSSIL ENERGY

Charles McConnell | University of Houston

Executive Director for Carbon Management and Energy Sustainability

The Honorable Charles McConnell joined the University of Houston Energy program in 2018 as the Executive Director for Carbon Management and Energy Sustainability. He coordinates a campus-wide effort to address marketplace challenges in the energy industry. Prior to joining UH Energy, Mr. McConnell was the executive director of the Energy and Environment Initiative at Rice University for the past 5 years.

Mr. McConnell served as the Assistant Secretary of Energy in the US Department of Energy from 2011-13 and was responsible for the Office of Fossil Energy's strategic policy leadership, budgets, project management, and research and development of the department's coal, oil and gas, and advanced technologies programs, as well as for the operations and management of the U.S. Strategic Petroleum Reserve and the National Energy Technologies Laboratories.

From 2009-11, Mr. McConnell served as Vice President of Carbon Management at Battelle Energy Technology in Columbus, Ohio. The initial 32 years of McConnell's career were with Praxair, Inc. serving in a variety of operations, sales and global business and technology roles including hydrogen, gasification and energy as the Global VP of Energy and Hydrogen. Assignments also included an ex-pat posting in Singapore for Asia business.

Mr. McConnell currently serves on the US EPA Science Advisory Board, is a board member of the Energy & Environmental Research Center (EERC) Foundation in North Dakota, is a member of the National Coal Council, has served on the Society of Petroleum Engineers and National Petroleum Council subcommittees, and has held a number of board positions including chairmanships of the Gasification & Syngas Technologies Council and the Clean Carbon Technology Foundation of Texas. Mr. McConnell holds a bachelor's degree in chemical engineering from Carnegie Mellon University (1977) and an MBA in finance from Cleveland State University (1984).

KEYNOTE, QUANTUM INFORMATION SCIENCE

Celia Merzbacher, Ph.D. | Quantum Economic Development Consortium

Associate Director of the Quantum Economic Development Consortium (QED-C)

Dr. Celia Merzbacher is the Associate Director of the Quantum Economic Development Consortium (QED-C), a recently created consortium that aims to enable and strengthen the U.S. commercial quantum industry. QED-C is supported by the National Institute of Standards and Technology (NIST) and more than 70 industry members and is managed by SRI International.

Prior to joining SRI, Dr. Merzbacher was Director of Institutional and Strategic Planning at Oak Ridge National Laboratory and served as Vice President for Innovative Partnerships at the Semiconductor Research Corporation. In 2003-2008, she was Assistant Director for Technology R&D and Executive Director of the President's Council of Advisory on Science and Technology (PCAST) in the White House Office of Science and Technology Policy. She began her career as a materials scientist at the U.S. Naval Research Laboratory.

BIOS: PANEL-1

PANEL 1 – QUANTUM SENSORS/DETECTORS AND QUANTUM EXPERIMENTS

Randall W. Gentry, Ph.D. | National Energy Technology Laboratory

Deputy Director, and Chief Research Officer, Science and Technology Strategic Plans and Programs

Dr. Randall Gentry has more than 20 years' experience in environmental science and engineering with a focus on water resources. He came to NETL after serving as Deputy Division Director of the Argonne National Laboratory's Environmental Science Division. He has also served as an associate editor of the Journal of Hydrologic Engineering and was a tenured faculty member at the University of Tennessee for more than 9 years. During that time, he held senior leadership positions overseeing the technology transfer operation for the University and led the State's Higher Education Centers of Excellence in Energy and Environment.

Dr. Gentry's research career has focused on the intersection of science and engineering with a goal of attaining a better understanding and ability to better characterize complex system behavior using computational techniques and tracer techniques. Dr. Gentry earned his Ph.D. and M.S. in civil engineering from the University of Memphis, and a B.S. in civil engineering from Memphis State University.

Prior to joining Argonne National Laboratory, Dr. Gentry begun federal service as Director of Environmental Sciences Division with the National Exposure Research Laboratory in the Office of Research and Development at the U.S. Environmental Protection Agency.

Chethan Acharya, Ph.D. | Southern Company

Principal Engineer at Southern Company Services

Dr. Chethan Acharya is a principal engineer in Southern Company Research and Development (R&D). He leads fossil fleet modernization research as part of the Generating Fleet R&D team. He also supports gas pipeline R&D in conjunction with Southern Company Gas.

Since joining Southern Company in 2011, Chethan has developed research strategies and evaluated carbon capture, Mercury and Air Toxics Standards (MATS) and Effluent Limitations Guidelines (ELGs) technologies. He also supported Alabama Power's 25-megawatt carbon capture project. Recently, his focus has shifted to plant modernization for O&M cost reduction and flexible operations. He is developing digital technologies such as advanced controls, sensors and analytics.

Chethan also collaborates directly with external organizations, like the Electric Power Research Institute (EPRI) and the U.S. Department of Energy. He serves as the advisor for EPRI's instrumentation, controls, and automation research program. Under this program, his primary initiative is developing an infrastructure to enable digital transformation at power plants. He is a member of NYSEARCH, where he influences gas pipeline R&D programs. Chethan received his B.S. in Chemical Engineering from Madras University in India and Ph.D. in Chemical Engineering from the University of Alabama. After graduation, he worked as a Postdoctoral Scholar at University of California at San Diego, where he focused on biomass gasification for power generation and liquid fuel production.

Henry Du, Ph.D. | Stevens Institute of Technology

Professor of Materials Science & Engineering

Dr. Henry Du is the Associate Dean for Research in the Schaefer School of Engineering and Science and Professor of Materials Science & Engineering at Stevens Institute of Technology. In addition to providing leadership for the research enterprise in the Schaefer School, Dr. Du is also actively engaged in federally funded research and doctoral student training.

Dr. Du's research focuses primarily on specialty optical fiber and fiber sensors; size- and shape-controlled synthesis of plasmonic nanostructures; and molecular self-assembly of stimuli-responsive polyelectrolyte thin films. Target areas of applications include chemical and biological sensing and disease diagnosis; process monitoring in micro-reactors and energy production systems; and nanomedicine.

Dr. Du has published over 150 papers and holds four US patents. He was twice the recipient of the Jess Davis Memorial Award for research excellence at Stevens and a recipient of the NSF Research Initiation Award. Dr. Du is a Fellow of SPIE.

BIOS: PANEL-1

Benjamin Gilbert, Ph.D. | Lawrence Berkeley National Laboratory

Senior Scientist

Dr. Benjamin Gilbert is a Senior Staff Scientist at Lawrence Berkeley National Laboratory (LBNL) and Adjunct Associate Professor in the Department of Earth and Planetary Science at the University of California – Berkeley. At LBNL Dr. Gilbert directs an integrated Geoscience group, a multi-investigator project funded by the DOE Basic Energy Science studying fundamental rock-fluid interactions in subsurface energy and water systems. He leads a collaboration between LBNL and UC–Berkeley scientists to develop and translate quantum-sensing methods into practical instrumentation for geochemical analysis and imaging.

Dr. Gilbert is an experimental geochemist with expertise in molecular spectroscopy and chemical imaging methods that traverse the electromagnetic spectrum. He has made contributions in nanogeoscience— the study of the properties and geochemical interactions of natural nanoscale minerals—and the use of ultrafast spectroscopic methods to reveal the mechanism of geochemical reactions.

Dr. Gilbert obtained a B.A. in Natural Sciences (Physics) from Cambridge University in 1994 and a Ph.D. from the École Polytechnique Fédérale de Lausanne (EPFL) in 2000. In 2010, he was recipient of the Mineralogical Society of America - Young Investigator Award. He joined LBNLin 2004 and was promoted to Senior Scientist in 2017. From 2015-19 he held an invited professorship position at the Institut des Sciences de la Terre at the University of Grenoble.

Michael Hatridge, Ph.D. | University of Pittsburgh

Assistant Professor of Physics

Dr. Michael Hatridge is an assistant professor in the Department of Physics and Astronomy at the University of Pittsburgh. He is a leader in the development of parametric amplifiers and efficient quantum measurement. His current research focuses on remote quantum interactions via "flying" qubits.

He received a B.S. in physics from Texas A&M University in 2004 and a PhD in condensed matter physics from Berkeley in 2010. From 2010-2015 he was a postdoctoral associate in QLab at Yale University, working under the supervision of Michel Devoret. He is the recipient of the 2015 Michelson Postdoctoral Prize Lectureship.

Benjamin Lawrie, Ph.D. | Oak Ridge National Laboratory

Research Scientist in Quantum Information Science

Dr. Ben Lawrie is a research scientist in the Quantum Information Science group at ORNL and a joint assistant professor in the Bredesen Center at the University of Tennessee. He received his PhD in interdisciplinary materials science from Vanderbilt University in 2011 and has focused on experimental research in quantum sensing and quantum nanophotonics since then. His current research programs center on (1) milliKelvin optical and scanning probe microscopy of qubits, quantum sensors, and quantum materials, (2) optical and electron beam characterization of quantum nanophotonic systems, and (3) the development of practical squeezed quantum sensors.

Carl Williams, Ph.D. | National Institute of Standards and Technology

Deputy Director of the Physical Measurement Laboratory (PML)

Dr. Carl J. Williams is the Deputy Director of the Physical Measurement Laboratory (PML), National Institute of Standards and Technology (NIST). He is a Fellow of the Joint Quantum Institute, the Joint Center for Quantum Information in Computer Science, and Adjunct Professor of Physics at the University of Maryland.

Dr. Williams received his B.A. in Physics from Rice University in 1981, his Ph.D. from the University of Chicago in 1987, joined NIST in 1998. In 2006, Dr. Williams helped establish the Joint Quantum Institute (JQI). He is a Fellow of the American Physical Society, the American Association for the Advancement of Science, and the Washington Academy of Science. He is an Associate Editor of the Journal of Quantum Information and Computation, has authored over 120 scientific publications, and has been a speaker at numerous national and international conferences.

BIOS: PANEL-2

PANEL 2 – QUANTUM COMPUTATION FOR MACHINE LEARNING, AI, AND OPTIMIZATION

David Miller, Ph.D. | National Energy Technology Laboratory

Senior Fellow for Process Systems Engineering and Analysis

Dr. David Miller leads the Institute for the Design of Advanced Energy Systems (IDAES), a virtual organization with researchers from NETL, Sandia National Laboratory, Lawrence Berkeley National Laboratory, Carnegie Mellon University, and West Virginia University, that is developing next generation process systems engineering tools for the identification, synthesis, optimization and analysis of innovative advanced energy systems at scales ranging from process to system to market. Previously, he served as the Technical Director of the Carbon Capture Simulation Initiative (CCSI) where he provided the overall leadership to a virtual organization with an annual budget of $10 million, consisting of over 100 researchers from five national laboratories and five universities and a stakeholder group consisting of representatives of over 20 companies.

He led the successful development, demonstration, and deployment of the R&D 100 Award winning suite of computational tools and models. He recently led the transition of CCSI to a second phase which will apply the CCSI computational approaches to reduce technical risk while accelerating the scale up of new carbon capture technologies. In June 2015, he received the Arthur S. Flemming Award for Exceptional Federal Service, Applied Science and Engineering, in recognition of his leadership of CCSI and its accomplishments. Prior to joining NETL, Dr. Miller spent a decade in academia, rising to the rank of Associate Professor with tenure, while conducting research related to process modeling, optimization, and scale-up and teaching process design. Dr. Miller earned his Ph.D. in chemical engineering from The Ohio State University.

Michael Flatté, Ph.D. | University of Iowa

Professor at the University of Iowa

Dr. Michael E. Flatté (AB Physics, Harvard, 1988; PhD Physics, UCSB, 1992) is a professor at the University of Iowa (UI). His research interests include optical and electrical control of spin dynamics in materials, novel spintronic devices, quantum sensors, and solid-state realizations of quantum computation. After postdoctoral work at the Institute for Theoretical Physics at UCSB and at Harvard University, he joined the UI faculty in 1995. He directed UI's Optical Science and Technology Center 2010-2017. Flatté has more than 200 publications and 10 patents. He is a Fellow of the American Association for the Advancement of Science and of the American Physical Society (APS) and chaired the APS' Division of Materials Physics 2016-2017. In 2019, he developed the first course on Quantum Engineering for the Pritzker School of Molecular Engineering at the University of Chicago. Flatté also has an adjunct appointment as professor at Eindhoven University of Technology.

Aaron Hussey, P.E. | Integral Analytics

Founder & Principal

Mr. Aaron Hussey is the principal for Integral Analytics' business and consulting activities with an emphasis on power industry implementation of advanced pattern recognition (APR) models and analytics software design and prototyping. Current responsibilities include APR model development and program implementation for Ontario Power Generation (OPG) monitoring & diagnostic center under contract to WSC, Inc., assessment of critical sensors using a failure modes and effects analysis (FMEA) for large electric generators under contract to the Electric Power Research Institute (EPRI), and various analytics software design and prototyping efforts for software vendors and electric utilities covering nuclear, fossil-fuels, and hydroelectricity.

Before founding Integral Analytics, Aaron's responsibilities included implementation of predictive analytic models for Duke Energy's 11-unit fleet of nuclear power plants, Tennessee Valley Authority's (TVA) fossil, hydro, and nuclear generating units, and South Carolina Electric & Gas (SCE&G) VC Summer nuclear site. Prior to that, he fulfilled various roles over 9+ years at the Electric Power Research Institute, focusing on instrumentation and controls (both nuclear and non-nuclear) research including project management for the Fleet-Wide Monitoring Interest Group.

BIOS: PANEL-2

Zlatko Minev, Ph.D. | IBM

Research Staff Member

Dr. Zlatko K. Minev is a research staff member at IBM Quantum Research, based out of T.J. Watson. Minev received his Ph.D. with distinction from Yale University in the field of quantum computing, control, and information in the group of Michel Devoret. His dissertation research realized an experiment considered beyond the reach of experimental atomic physics, whose significance was summarized by Nature: "[The] experiment overturns Bohr's view of quantum jumps, demonstrating that they possess a degree of predictability and when completed are continuous, coherent and even deterministic." Dr. Minev received his B.A. from UC Berkeley with distinction and high honors. Dr. Minev's research is focused on circuit quantum electrodynamics (cQED), random circuits, ns-latency feedback control, stochastic trajectories, and quantum architectures, and has been featured in mainstream media worldwide (50+ news publications) and live interviews (e.g., NPR). In 2012, Minev founded and presently chairs a nationwide science outreach and career pathways organization (Open Labs).

Nick Sahinidis, Ph.D. | Carnegie Mellon

John E. Swearingen Professor and Director of the Center for Advanced Process Decision-making

Dr. Nick Sahinidis is the John E. Swearingen Professor and Director of the Center for Advanced Process Decision-making at Carnegie Mellon University. He joined Carnegie Mellon in 2007 after a sixteen-year long career at the University of Illinois at Urbana, where he taught in Industrial Engineering and Chemical Engineering. His research has included the development of theory, algorithms, and the BARON software for global optimization of mixed-integer nonlinear programs. Professor Sahinidis' research activities have been recognized by the INFORMS Computing Society Prize in 2004, the Beale-Orchard-Hays Prize from the Mathematical Programming Society in 2006, the Computing in Chemical Engineering Award in 2010, the Constantin Carathéodory Prize in 2015, and the National Award and Gold Medal from the Hellenic Operational Research Society in 2016. Professor Sahinidis is a fellow of INFORMS and AIChE. He is the Editor-in-Chief of *Optimization and Engineering*.

Earl Scime, Ph.D. | West Virginia University

Interim Dean of the Statler College of Engineering and Mineral Resources

Dr. Earl Scime is the interim dean of the Statler College of Engineering and Mineral Resources. Scime, the Jefimenko Professor of Physics and Astronomy, has been a member of the WVU faculty since 1995. He served as chair of physics from 2002-2019 and as the interim associate vice president for research.

Dr. Scime earned his B.S. in physics and applied mathematics from Florida State University and Ph.D. in plasma physics from the University of Wisconsin – Madison. Dr. Scime has received WVU's Benedum Award for Distinguished Scholarship, Foundation Outstanding Teaching Award, and the Heebink Award for Distinguished Service. He is a Fellow of the American Physical Society and has served as chair of the APS Division of Plasma Physics.

Dr. Scime's research interests include fusion energy, space and industrial plasma physics, plasma diagnostics, magnetic reconnection, robotics and STEM education. He has been recognized globally for his mentoring of students of all ages.

John D. Siirola, Ph.D. | Sandia National Laboratories

Principal R&D Member of Technical Staff in the Discrete Math and Optimization Department within the Center for Computing Research

Dr. John D. Siirola is a Principal R&D Member of Technical Staff in the Discrete Math and Optimization Department within the Center for Computing Research at Sandia National Laboratories. His main areas of expertise are systems design, operations research, optimization modeling, and optimization algorithms. John's research focuses on the intersection of computational tools, emerging computing platforms, and systems design and analysis; in particular, developing approaches for modeling highly structured systems, optimization algorithms that can exploit the expressed structure, and the application of these techniques to national security problems.

Dr. Siirola has a B.S. from Purdue University (2000) and Ph.D. from Carnegie Mellon University (2005), both in Chemical Engineering. He is a senior member of the AIChE, member of INFORMS, and member of the COIN-OR Foundation. John currently serves on the COIN-OR Technical Leadership Council and co-chaired the 2014 Foundations of Computer Aided Process Design (FOCAPD) conference.

BIOS: PANEL-3

PANEL 3 – QUANTUM COMPUTATION/SIMULATION FOR CHEMISTRY AND MATERIALS

Andrew Baczewski, Ph.D. | Sandia National Laboratories

Principal R&D Member of Technical Staff

Dr. Andrew Baczewski is a Principal Member of the Technical Staff in the Quantum Computer Science department at Sandia National Laboratories and an Adjunct Assistant Professor with the Center for Quantum Information and Control at the University of New Mexico. He received an interdisciplinary Ph.D. in physics and electrical engineering from Michigan State University in 2013, and has been with Sandia ever since. His research focuses on semiconductor quantum devices and all aspects of quantum simulation, particularly as it applies to problems in materials science and condensed matter physics.

Ignasi Palou-Rivera, Ph.D. | RAPID Manufacturing Institute

Technology Platform Director of the RAPID Manufacturing Institute

Dr. Ignasi Palou-Rivera is currently the Technology Platform Director of the RAPID Manufacturing Institute. RAPID is a collaboration between the US Department of Energy Advanced Manufacturing Office and AIChE on Modular Chemical Process Intensification (MCPI). Ignasi holds an Engineer degree from the Universitat Politècnica de Catalunya in Barcelona and a Ph.D. in Chemical Engineering from the University of Wisconsin-Madison. Ignasi's professional career spans the areas of process development, modeling and optimization; techno-economic, life-cycle, and sustainability analysis; and R&D management for a variety of organizations such as BP, LanzaTech and Argonne National Laboratory.

Raphael Pooser, Ph.D. | Oak Ridge National Laboratory

Senior Research Scientist

Dr. Raphael Pooser is an expert in quantum computing and continuous variable quantum information. His research interests include quantum computing, neuromorphic computing, and sensing. He currently leads the Quantum Computing Testbed Pathfinder project at ORNL, a large multi institution collaboration with a focus on benchmarking near-term quantum computers. Through this program Dr. Pooser has led the development of an array of application-inspired benchmarks for assessing the performance of currently available and near-term quantum computers. These benchmarks focus on metrics like accuracy of the computation, equivalent classical computational power of a given quantum circuit, sampling accuracy, and error reduction capabilities. Some of the benchmarks have led to dramatic improvements in the results for small algorithms, such as in quantum chemistry simulations, run on today's hardware.

Dr. Pooser has also developed a quantum sensing program from the ground up based on continuous-variable quantum networks over the past eight years at ORNL. His research model uses real-world, practical quantum sensors as a showcase for the technologies that will enable scalable quantum computing. Dr. Pooser has over 16 years of quantum information science experience. Prior to his post as senior research scientist, he served as a distinguished Wigner Fellow at ORNL. He previously worked as a postdoctoral fellow in the Laser Cooling and Trapping Group at NIST after receiving his Ph.D. in Engineering Physics from the University of Virginia. He received a B.S. in Physics from New York University.

BIOS: PANEL-3

Philip Richerme, Ph.D. | Indiana University

Assistant Professor of Physics

Dr. Phil Richerme is an Assistant Professor of Physics at Indiana University. His current research focuses on the development of two-dimensional (2D) arrays of trapped ions, which serve as a well-isolated platform for experimental quantum information processing. Applications of his research include the creation and study of exotic 2D quantum materials as well as the quantum simulation of quantum chemical systems. He received his Ph.D. from Harvard University in 2012, under the direction of Gerald Gabrielse, followed by postdoctoral research with Chris Monroe at the Joint Quantum Institute/University of Maryland.

Mike Santos, Ph.D. | University of Oklahoma

Professor of Physics and the Charles L. Blackburn Chair in Engineering Physics

Dr. Michael Santos is a Professor of Physics and the Charles L. Blackburn Chair in Engineering Physics at the University of Oklahoma, where he has worked since 1993. His research focuses on the growth of III-V semiconductors by molecular beam epitaxy and the application of these materials as sensors, optoelectronic devices, and platforms for studying quantum effects. His research has been supported by the NSF, DoD, DOE, and the semiconductor industry.

Dr. Santos has been a visiting professor at Tohoku University and NTT Basic Research Laboratories in Japan. He was a postdoctoral researcher at AT&T Bell Laboratories, received a Ph.D. from Princeton University, and received a B.S. degree from Cornell University. In 2012, Prof. Santos was elected as a Fellow of the American Physical Society for growth of compound semiconductor nanostructures and spin transport. He has co-authored more than 200 papers on experimental semiconductor research.

Götz Veser, Ph.D. | University of Pittsburgh

Nickolas DeCecco Professor of Chemical Engineering

Dr. Götz Veser is the Nickolas DeCecco Professor of Chemical Engineering at the University of Pittsburgh. He obtained a Diploma in chemical engineering from the University of Karlsruhe, and a PhD in physical chemistry from the Fritz Haber Institute, Berlin (Germany). Following a Feodor-Lynen Postdoctoral Fellowship at the University of Minnesota, he held positions at the University of Stuttgart and at the Max-Planck-Institute for Coal Research, before joining the University of Pittsburgh in 2002.

Dr. Veser's research interests focus on catalytic reaction engineering, functional nanomaterials, and process intensification, with applications that span from clean energy production, carbon capture, and fuels processing, to production of specialty chemicals. He serves on the editorial board of multiple reaction engineering journals, as Science Ambassador for the National Academies of Science and Engineering, on the Governing Board for AIChE-RAPID, the Executive Council for NETL-UCFER, and the board of the North American Catalysis Society.

BIOS: PANEL-4

PANEL 4 – QUANTUM COMPUTATION FOR PROCESS MODELING/CFD AND QUANTUM NETWORKING

Richard Bajura, Ph.D. | West Virginia University

Director Emeritus, National Research Center for Coal and Energy (NRCCE)

Dr. Richard Bajura served in multiple roles at West Virginia University during his 50 year career as a faculty member and research administrator. For the past 35 years, he facilitated, lead, and managed energy and environment programs in research and technical outreach with WVU faculty and with external organizations in his leadership role in WVU's National Research Center for Coal and Energy. Bajura retired as the NRCCE Director in 2017, and currently holds the titles of NRCCE Director Emeritus and Acting Director of the Energy Institute's US-China Energy Center. His current assignments include technology development and outreach in fossil energy applications in the US and in building collaborative research and academic program initiatives with counterparts in Chinese universities and industrial organizations.

Dr. Bajura remains active on the ASME Energy Committee, the National Coal Council, the Carbon Utilization Research Council (CURC), the Pittsburgh Coal Conference Advisory Board, and the Washington Coal Club Board of Directors. He participates as the group leader for the fuels and crosscutting research programs of the CURC Technical Committee developing technology road maps for national coal R&D programs and as an executive committee member for the oil and natural gas programs of the Research Partnership to Secure Energy for America (RPSEA).

Joseph Berry, Ph.D. | The National Renewable Energy Laboratory**

Senior Scientist, Perovskite and Hybrid Solar Cells Team Lead

Dr. Joseph Berry is a senior research scientist at NREL. He received his doctorate in physics from Penn State University in 2001. His thesis work focused on semiconductor spintronics with an emphasis on coherent spin transport across interfaces, spin polarized transport in 2-DEGs, and development of hybrid ferromagnetic semiconductor materials. Much of this work is foundational to efforts in the field of spintronics. From 2001 to 2007, he worked as a postdoctoral researcher at the National Institute of Standards and Technology in Boulder, Colorado, specializing in development and application of narrow band spectroscopies to the studies of III-V quantum dots.

From 2007 to the present, Dr. Berry has worked as a scientist at NREL on oxide semiconductor systems with a focus on both basic materials physics and device applications of these materials.

In addition to his position at NREL, Dr. Berry is an affiliate of the Renewable and Sustainable Energy Institute and a lecturer in the Department of Physics at the University of Colorado at Boulder.

Stephen F. Bush, Ph.D. | GE Global Research Center

Senior Scientist in Algorithmic Communications Network Theory

Dr. Stephen F. Bush is a Senior Scientist in Algorithmic Communications Network Theory at the GE Global Research Center. Dr. Bush was presented with a Gold Cup Trophy Award from DARPA for his work in fault tolerant networking. Stephen F. Bush received the B.S. degree in electrical and computer engineering from Carnegie Mellon University, M.S. degree in computer science from Cleveland State University, and Ph.D. degree from the University of Kansas. He is the author of Smart Grid: Communication-Enabled Intelligence for the Electric Power Grid (Wiley – IEEE, 2014) and Nanoscale Communication Networks (Norwood, MA: Artech House, 2010).

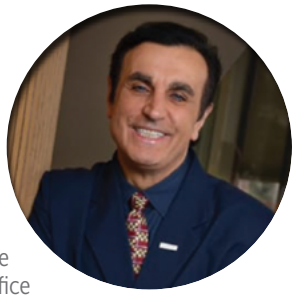
Dr. Bush coauthored a book on active network management, titled Active Networks and Active Network Management: A Proactive Management Framework (New York, NY: Kluwer Academic/Plenum Publishers, 2001). Dr. Bush is the past chair of the IEEE Emerging Technical Subcommittee on Nanoscale, Molecular, and Quantum Networking and currently chair for the IEEE 1906.1 standards working group on nanoscale communication networks. Dr. Bush is an IEEE Distinguished Lecturer on the smart grid and nanoscale communication networks. He taught Quantum Computation and Communication at Rensselaer Polytechnic Institute and is leading an effort to start IEEE P1913, Software-Defined Quantum Communication.

**Panelist was unable to attend the workshop.

BIOS: PANEL-4

Peyman Givi, Ph.D. | University of Pittsburgh

Distinguished Professor of Mechanical Engineering and the James T. MacLeod Professor in Swanson School of Engineering



Dr. Peyman Givi is Distinguished Professor of Mechanical Engineering and the James T. MacLeod Professor in Swanson School of Engineering at the University of Pittsburgh. Previously he held the rank of University Distinguished Professor in Aerospace Engineering at the State University of New York at Buffalo, where he received the Professor of the Year Award by Tau Beta Pi (2002). He also worked as a Research Scientist at the Flow Industries, Inc. in Seattle. Dr. Givi has had frequent visiting appointments at the NASA Langley & Glenn (Lewis) centers, and received the NASA's Public Service Medal (2005). He is amongst the first 15 engineering faculty nationwide who received the White House Presidential Faculty Fellowship from President George Bush. He also received the Young Investigator Award of the Office of Naval Research, and the Presidential Young Investigator Award of the National Science Foundation.

Dr. Givi is the Deputy Editor of AIAA Journal, member of the editorial boards of Computers & Fluids, Journal of Applied Fluid Mechanics; the Open Aerospace Engineering Journal, an Associate Editor of Journal of Combustion; and a past advisory board member of Progress in Energy and Combustion Science. He received his Ph.D. from the Carnegie Mellon University (PA), and BE (Summa Cum Laude) from the Youngstown State University (OH), where he was named the 2004 Phi Kappa Phi Distinguished Alumnus, and the 2012 STEM College Outstanding Alumnus. Dr. Givi has achieved Fellow status in AAAS, AIAA, APS, and ASME; and was designated as ASME's Engineer of the Year 2007 in Pittsburgh.

Supratik Guha, Ph.D. | Argonne National Laboratory*

Joint Appointment/Senior Advisor to PSE

Dr. Supratik Guha is senior advisor to the Physical Sciences and Engineering directorate, leading Argonne's microelectronics and quantum information science strategic efforts. He is also a professor at the Pritzker School of Molecular Engineering at the University of Chicago.

Dr. Guha led the Center for Nanoscale Materials, a U.S. Department of Energy Office of Science user facility, from 2015 to 2019. Before joining Argonne and the University of Chicago in 2015, he spent twenty years at IBM Research where he last served as the Director of Physical Sciences. At IBM, Dr. Guha pioneered the materials research that led to IBM's high dielectric constant metal gate transistor, one of the most significant developments in silicon microelectronics technology. He was also responsible for initiating or significantly expanding IBM's R&D programs in silicon photonics, quantum computing, sensor based cyberphysical systems and photovoltaics.

Dr. Guha is a member of the National Academy of Engineering and a Fellow of the Materials Research Society, American Physical Society, a 2018 Department of Defense Vannevar Bush Faculty Fellow, and the recipient of the 2015 Prize for Industrial Applications of Physics. He received his Ph.D. in materials science in 1991 from the University of Southern California, and a B.Tech in 1985 from the Indian Institute of Technology, Kharagpur. At the University of Chicago and Argonne, his interests are focused on discovery science in the area of nano-scale materials and epitaxy for energy, sensing and future information processing.

Ahmad H. Haidari, Ph.D. | ANSYS**

Global Industry Director at ANSYS Inc.

Dr. Ahmad H. Haidari is the global industry director for the Energy, Process & Power industry segments at ANSYS, Inc. He has close to 30 years of experience in the application of engineering simulation and modeling technology to product development processes. In this position he is responsible for ensuring that the full portfolio of ANSYS engineering simulation software meet the modeling and simualtion requriments of organziations working on topics related to energy, electrification, power generation and process industries.

Dr. Haidari received his Ph.D. in 1989 from Lehigh University in Bethlehem, PA, in Mechancial Engineering with conceration in Thermo-Fluid Scinces. He has worked or has been invovled with experimental and computional physics realted to fluids since the early 1980s.

Michael Leuenberger, Ph.D. | University of Central Florida

Professor, Department of Physics

Dr. Leuenberger received his PhD in Theoretical Condensed Matter Physics from the University of Basel, Switzerland. He spent three years as a postdoctoral associate in three different institutions (University of California San Diego, University of Iowa, University of Basel Switzerland) before joining UCF in 2005 as an assistant professor.

*Panelist was moved to panel 1.
**Panelist was unable to attend the workshop.

FOSSIL ENERGY WORKSHOP ON

QUANTUM INFORMATION SCIENCE & TECHNOLOGY

NOVEMBER 19–20, 2019
NATIONAL ENERGY TECHNOLOGY LABORATORY
PITTSBURGH, PA

U.S. DEPARTMENT OF ENERGY | Office of Fossil Energy

NATIONAL ENERGY TECHNOLOGY LABORATORY

1450 Queen Avenue SW
Albany, OR 97321
541-967-5892

3610 Collins Ferry Road
P.O. Box 880
Morgantown, WV 26507
304-285-4764

626 Cochrans Mill Road
P.O. Box 10940
Pittsburgh, PA 15236
412-386-4687

Program staff are also located in
Houston, TX and **Anchorage, AK**

CUSTOMER SERVICE
1-800-553-7681

www.NETL.DOE.gov