Lawrence Berkeley National Laboratory

Status of the FY20 LBNL LDRD Program

The LDRD program at Berkeley Lab continues to produce cutting edge research for DOE and the nation. For the FY20 cycle, with 168 total proposals submitted, the response to the LDRD Call for Proposals remains strong. The Lab's scientific leadership reviewed each proposal under one of three funding tracks: Lab Initiative, Area Priority, or Early Career Development. The projects chosen for funding under the Lab Initiative track fell under one of five topics: Beyond Moore's Law, Genetically Encoded COmposites (GECO), Machine Learning for Science, Solid State Energy Storage, and the Water-Energy Nexus. Berkeley Lab has also been recognized by DOE for its Early Career Development (ECD) track, which targets candidates no more than seven years removed from their Ph.D. FY20 is the third annual cohort for this track. Finally, Area Priority projects were selected with input from each proposal's direct Division and Associate Lab Director with focus on topics that were of significant and targeted relevance to their Divisions and Area. A list of all FY20 LDRD projects and PIs is included on pages four and five, with notations for Lab Initiatives and ECD projects.

The Lab has funded 96 LDRD projects for FY20 at a total value of $23.0M. This represents an increase of approximately $1M from FY19 levels.

Beyond Moore's Law

The world has long known that the physical limits of transistor engineering would one day be reached. This would be a significant setback for much of the research being conducted by DOE, whose needs will only grow more significant as it moves further into the future. To solve this issue, Berkeley Lab is challenged to reimagine the digital computing paradigm starting from new materials, physical concepts, and new architectures to novel technologies with new functionalities that could lead to unprecedented computing efficiency.

Originally proposed in FY2017 as part of the Exploration of Novel Computing Technologies initiative, Beyond Moore's Law projects have received $3.5M of funding to date.

Genetically Encoded COmposites

Living organisms produce a variety of biominerals composed of soft and hard materials, including bone, shells, and exoskeletons. These composites, whose synthesis and morphology is genetically-encoded, are created in an energy-efficient manner and are frequently hierarchically-structured, yielding properties superior to traditional materials. This initiative aims to discover existing genetically-encoded

composites, understand their synthesis and structure-function relationships, and leverage this new knowledge to produce non-natural composites with improved function.

This initiative's initial project received $233,000 for FY20.

Machine Learning for Science

Tying closely to the physical aspects addressed in the Beyond Moore's Law initiative, Machine Learning for Science is approaching the hurdles of next generation computational speed and analytical techniques from programming, statistical, and mathematical methods. Such methods include dimensionality reduction, clustering, regression, optimization and inference, along with deep learning methods that have proven effective on speech and image data.

Initially proposed for FY18, the Machine Learning for Science LDRDs have received $4.1M through FY20.

Solid State Energy Storage

Solid state systems are an exciting area of exploration for safe, high energy density batteries. LBNL is addressing the critical science of solid state batteries, including modeling, design and synthesis of novel solid-state conductors and their integration into membranes, modeling and characterization of reactivity at buried interfaces, and innovative new processing methods of integrated electrodes and complete solid-state batteries.

Also new for FY20, Solid State Energy Storage projects have received an initial total funding value of $1.2M.

Water-Energy Nexus

Water sourcing issues are ever-present in California, and in cities and nations across the globe. The primary goal of the Water-Energy Nexus is to tackle impediments affecting clean water availability, production costs, and resiliency against natural events. Of importance to the Department of Energy, water is a critical requirement for power generation, and water treatment is a major user of electrical power in the United States. While innovations in energy production, storage and efficiency have led to dramatic improvements in the stability of the U.S. energy sector, water is increasingly becoming the unstable element. Berkeley Lab scientists are pioneering a range of new technologies and systems to reduce the cost, and improve the reliability of U.S. water production.

Initially begun during the FY17 LDRD cycle, $5.4M in Water-Energy Nexus projects have highlighted the independent research being conducted that helped support Berkeley Lab's proposal for the recently awarded $100M DOE innovation hub.

Early Career Development

The Early Career Development (ECD) track's intent is to provide financial support and stability to the next generation of talented scientists and researchers at Berkeley Lab. During the FY17 LDRD review cycle, the Lab's Division Directors, ALDs, and senior Directorate staff identified a disconnect in the transition period between when a promising early career scientist is working in another PI's lab to that researcher becoming an independent scientist and PI themselves. Without PI or group lead experience, it is difficult to achieve research independence so that they can successfully request a DOE Early Career Award or other programmatic funding. The intent of the LDRD ECD track is to provide a financial runway to allow these candidates a two-year period to work on ideas they can turn into proposals for either direct DOE programmatic funding or the DOE Early Career Award program. For FY20, six new PIs in addition to the six continuing from FY19 were awarded a maximum of $225,000 each in pre-overhead LDRD funding. An equivalent amount is earmarked for year two of the FY20 cohort in FY21. An additional six to nine candidates are expected to join the six continuing PIs for FY21.

For more information related to the FY21 LDRD application process and scheduled deadlines, please visit the Lab's LDRD webpage at: https://www2.lbl.gov/DIR/LDRD/index.html. Proposals are due into the online submission database by March 23rd.

FY 2020 Lawrence Berkeley National Laboratory LDRD Projects

Division	Project Title	PI	Total Funding
AA	Fixed Field Magnets for Large Momentum Acceptance Transport of Ions	Brouwer,Lucas	$251,000
AA	Compact Laser-Based Positron Creation, Capture, and Cooling	Bulanov,Stepan	$153,000
AA	Deep Learning Based Control for Ultrafast Lasers and Accelerators	Du,Qiang	$288,000
AA	A Self-Switching Metal-Insulator Coating for the Quench Protection of High-Temperature Superconducting Magnets	Ji,Qing	$179,000
AA	Designing Radio Frequency Cavity with Multi-Objective Genetic Algorithm	Luo,Tianhuan	$182,000
AA	Qubit Synthesis Far From Equilibrium	Schenkel,Thomas	$248,000
AL	Correlation of Structural and Chemical Processes at Interfaces Under Operating Conditions Using Multimodal Ambient Pressure X-ray Photoelectron Spectroscopy and Surface X-ray Scattering	Nemsak,Slavomir	$178,000
AL	"Q/X-LAB": A System for Algorithmically Driven Synthesis of Quantum Materials Using X-ray Spectroscopy	Rotenberg,Eli	$276,000
AL	Developments and Integration of Theory for Advanced Spectroscopy of Electrochemistry	Yang,Wanli	$153,000
BE	Unnatural Biosynthetic Pathways by Combining Natural Pathways with Artificial Metalloenzymes (ArMs)	Keasling,Jay D	$322,000
BE	Closed-Loop Plastics from Biogenic Feedstocks	Keasling,Jay D	$196,000
BE	Electron Economical CO2 Bioconversion	Singer,Steven W	$300,000
BE	Laser-Accelerated Ion Beams: Evaluating Radiobiological Effects	Snijders,Antoine M	$285,000
BE	Developing New Hosts to Enable Effective Electrons-to-Biomass Conversion	Sundstrom,Eric	$262,000
BU	AlphaBuilding: Machine Learning Based Advanced Building Controls	Hong,Tianzhen	$194,000
BU	Building Science-Based Methods to Quantify and Fortify Energy Resilience in Buildings	Mathew,Paul A	$129,000
BU	Managing Water Use to Reshape Electricity Loads: A User-Oriented Approach	Rao,Prakash	$255,000
CE	VISIBLE: Volatile Inference of Subsurface Interactions and the BiogeochemicaL Environment	Chakraborty,Romy	$197,000
CE	UAV-Mounted Passive ElectroMagnetic (EM) Sensor for Spatiotemporal Imaging of Shallow Subsurface Properties	Dafflon,Baptiste	$190,000
CE	Climate and Hydrological Controls on Coastal Algal Blooms	Newcomer,Michelle E	$280,000
CE	Process-Based Urban Hydro-Climate Modeling: Applications for Flood Risk Management and Ground Water Recharge in Cities	Vahmani,Pouya	$254,000
CE	Toward Accurately Predicting California Hydroclimate by Cracking the Tropical Storm King	Yang,Da	$307,000
CH	Ultrafast Science Beyond Pump-Probe: Reconstructing Chemical Dynamics from Temporal Correlations in Multi-Pulse X-ray Spectroscopy	Gessner,Oliver	$215,000
CH	Ionic Transport in Nanoconfined, Far-From-Equilibrium Fluids	Limmer,David T	$121,000
CH	The Duality of f-Electron Localization and Covalency in Lanthanide and Actinide Organometallics	Minasian,Stefan George	$149,000
CH	In-situ Investigation of Chemical PrecursorTransformation: Towards a Predictive Science of Synthesis	Sutter-Fella,Carolin Maria	$54,000
CR	Preparing the TOAST Cosmic Microwave Background High Performance Computing Framework for CMB-S4 Data Synthesis and Reduction on NERSC-9	Borrill,Julian	$341,000
CR	The Chemical Universe Through the Eyes of Generative Adversarial Neural Networks	de Jong,Wibe Albert	$161,000
CR	Multi-Tiered Iterative Projection Algorithms for Solving Inverse Problems for Imaging and Machine Learning	Donatelli,Jeffrey John	$287,000
CR	Deep Reinforcement Learning for NP-Complete Graph Problems in Scientific Computing	Ghysels,Pieter	$226,000
CR	Machine Learning through the PDE Lens: Design, Interpretability, and Efficiency	Minion,Michael Lee	$232,000
CR	Machine Learning with Advanced Feature Descriptors	Morozov,Dmitriy	$215,000
CR	Enabling Water-Energy Decision Support Using Watershed-Scale Surrogate Models	Mueller,Juliane	$324,000
CR	New Multiphysics Modeling of Next-Generation Electronic Devices	Ng,Esmond G	$223,000
CR	Network Dynamical Mechanisms Underlying Flexible and Self-Organized Brain Function	Nugent,Peter E	$233,000
CR	Combining Probabilistic Graphical Models and Deep Learning to Advance Scientific Data Analysis	Perciano Costa Leite,Talita	$292,000
CR	Energy Efficient Electronics for the Era Beyond CMOS: Post-Moore Architecture and Device Level Simulation	Shalf,John M	$283,000
CR	Building and Benchmarking a Modular Deep Learning Framework for Encoding and Decoding 3D Geometry of Atomic Systems	Smidt,Tess	$131,000
CR	SIFER - Scalable Data Infrastructure for in-Field Experimental Instruments	Tull,Craig	$181,000
CR	Approximate Unitary Matrix Decompositions for Quantum Circuit Synthesis	Van Beeumen,Roel Maria Franciscus	$288,000
CR	Network Computing for Experimental and Observational Data Management	Weber,Gunther Heinz	$194,000
CR	Statistical Mechanics for Interpretable Learning Algorithms	Wu,Kesheng	$322,000
EA	Big Data Fusion for Smart and Sustainable Mobility	Gonzalez,Marta	$286,000
EA	Emerging TechnoEconomic Analysis	Scown,Corinne Donahue	$252,000
EA	A Neuroeconomics Experiment to Study Routine Transportation Decision-Making Processes and Drivers	Spurlock,Cecily Anna	$139,000
EA	Breakthrough High-performance Computational Solutions to Secure a Reliable EV-connected Grid Future	Wang,Bin	$285,000
EB	Developing Third-Wave Machine Learning for the Biosciences	Brown,James Bentley	$633,000
EB	Roots 2.0: Reimagining a Root System Optimized for Plant-Microbe Interactions	Mortimer,Jennifer Charlotte	$279,000
ED	HEATER (Highly Efficient Advanced Thermal Energy Research) for On-Demand Thermal Energy	Dames,Christopher	$297,000

ED	Low-Temperature Solution-Phase Synthesis of Sulfide Glass Composite Solid Electrolytes	Liu,Gao	$284,000
ED	Enabling Scalable High Temperature Energy Conversion and Storage with Novel Optical Spectroscopy	Lubner,Sean	$285,000
ED	The Materials Project and Device Scale Modeling for Discovery of Novel Semiconductor Materials	Persson,Kristin Aslaug	$282,000
ED	Platform for Services Exchange at the Edge of Low Inertia Grids	Poolla,Kameshwar	$129,000
ED	Ion-Selective Inorganic Materials for Aqueous Environments	Subban,Chinmayee	$38,382
ED	Precision Manufacturing and Advanced Characterization of Optimized Solid-State Battery Components	Tucker,Michael C	$229,000
EG	Miniature Scanning Electron Beam Magnetic Probe	Turqueti,Marcos de Azambuja	$187,000
GO	Pore-scale Investigation of Fracture Alteration in Multiphase Systems	Deng,Hang	$281,000
GO	Geoscience Quantum Sensing	Gilbert,Benjamin	$292,000
GO	Ptychography of Diatoms	Gilbert,Pupa	$291,000
GO	Extended Finite Volume Method for Coupled Processes in Complex Fractured Geological Systems	Hu,Mengsu	$292,000
GO	Isotopic Constraints on the Chemical and Thermal Conditions of Thermogenic Methane Formation	Stolper,Daniel Aaron	$128,000
JG	Improving Bioenergy Yield Under Drought Stress from Field to Lab	Singer,Esther	$238,000
JG	Microbiology of Produced Water Recycling and Reuse	Tringe,Susannah Green	$244,000
JG	Developing a Biological 3D Fabrication Platform for Synthesis of Complex Genome-Encoded Composites	Yoshikuni,Yasuo	$233,000
MB	Characterization of Biological "Dark Matter" Communities Through Integration of Metagenomics and Cryo-Et Imaging	Davies,Karen Michelle	$312,000
MB	Developing High-Resolution Optical Microscopy Methods for Imaging Plants and Microbes	Ji,Na	$277,000
MB	Computational Tools for Extracting Macromolecular Conformational Dynamics from Diffraction and Imaging Data	Pande,Kanupriya	$284,000
MB	Engineering of Highly Selective Advanced Biogenics for Detection, Binding, and Control of Metal in the Environment	Ralston,Corie	$229,000
MB	Interactive Machine Learning for Tomogram Segmentation and Annotation	Sauter,Nicholas K	$155,000
MF	Solving Experimental Limitation to Implementations of Superconducting Qubits	Cabrini,Stefano	$243,000
MF	Ultrastable Superconducting Electron Microscope	Denes,Peter	$228,000
MF	Organo-Ionic (ORION) Frameworks as Solid-Ion Conductors with Tunable Chemomechanical Properties for Solid-State Batteries	Helms,Brett A	$277,000
MF	Tuning Interactions at Atomically Precise Interfaces for Controlling Quantum Coherent Phenomena in Nanoscale	Raja,Archana	$286,000
MF	Atomic Electron Tomography of Disordered Materials	Scott,Mary Cooper	$93,000
MF	Modeling and Characterization of the Composite Cathode and Solid Electrolyte for All Solid-State Batteries	Scott,Mary Cooper	$241,000
MF	Design, Synthesis, and Spectroscopic Studies of Photoactive MOFs for Solar Fuel Production	Zhang,Jian	$145,000
MS	Growth and In situ Characterization of Anisotropic 2D Layers and Heterostructures	Al Balushi,Zakaria Y	$146,000
MS	Novel Electronic Nanostructured Materials for Low Power Electronics	Fischer,Peter	$284,000
MS	Computational Design of Next Generation Materials for Quantum Sensing and Detection	Griffin,Sinead Majella	$275,000
MS	Ultrafast Electron Diffraction Studies of Quantum Materials	Kaindl,Robert	$383,000
MS	Investigation of Interphase Formation Between Solid-State Electrolyte and Metal Anode	Kim,Haegyum	$189,000
MS	Agile Hybrid Materials for a Sustainable Future	Lanzara,Alessandra	$281,000
MS	Understanding Fundamental Scientific Challenges in Scaling New Low Power Electronic Materials and Devices	Naulleau,Patrick P	$284,000
MS	Spatial-Temporal Imaging of Dirac Electron Dynamics	Wang,Feng	$303,000
NE	DFT Beyond Moore's Law: Extreme Hardware Specialization for the Future of HPC	Shalf,John M	$277,000
NS	Enabling A Ton-Scale Ge-76 Neutrinoless Double-Beta Decay Experiment	Barton,Paul Joseph	$268,000
NS	Extracting Quantum-Level Laws by Explainable Machine Learning and Automated Experiment Design	Lai,Yue Shi	$280,000
NS	Deep-Cryogenic CMOS ASIC development	Mei,Yuan	$349,000
NS	Developing New Lattice QCD Methods for Neutrinoless Double Beta Decay and Nuclear Physics	Walker-Loud,Andre	$229,000
PH	LightPix: Highly-Scalable Cryogenic SiPM Readout Electronics for Neutrino Physics	Dwyer,Daniel A	$219,000
PH	Charm Physics with ATLAS: From Charm Tagging to Z+c Measurements and Constraints on the Charm PDF	Gray,Heather Mary Audrey	$127,000
PH	Fiber Robot R&D for Next Generation Dark Energy Research	Schlegel,David J	$184,000
PH	Combining Data Driven and Science Based Generative Models	Seljak,Uros	$122,000
PH	Development of Integrated Frequency Domain Multiplexed Readout System for Next-generation Cosmic Microwave Background and Light Dark Matter Search Experiments	Suzuki,Aritoki	$244,000
PH	Exploring the Unknown Using the Higgs Boson with the ATLAS Experiment at the LHC	Wang,Haichen	$128,000
SN	FPGA Based Network Processor Architectures and Applications Research.	Guok,Chin	$277,000

Denotes a Lab Initiative Project

Denotes an Early Career Development Project

Divisional Key

AA Accelerator Technologies and Applied Physics

AL	Advanced Light Source
BE	Biological Systems and Engineering
BU	Building Technologies and Urban Systems
CE	Climate and Ecosystem Sciences
CH	Chemical Sciences
CR	Computational Research
EA	Energy Analysis and Environmental Impacts
EB	Environmental Genomics and Systems Biology
EG	Engineering
ED	Energy Storage and Distributed Resources
GO	Energy Geosciences
JG	Joint Genome Institute
MB	Molecular Biophysics and Integrated Bioimaging
MF	Molecular Foundry
MS	Materials Sciences
NE	NERSC
NS	Nuclear Science
PH	Physics
SN	Scientific Networking