QC^3 Project Descriptions

Quantum Computing for Computational Chemistry

The Boeing Company – Arlington, VA

QUantum Innovation for Corrosion Kinetics (QUICK) - $2,509,300

Boeing aims to develop a new method for modeling material corrosion (i.e., rust). The team seeks to improve material durability across a range of aerospace, steel, and electric battery applications. They aim to deliver corrosion rate predictions up to 100x faster and more accurate than state-of-the-art approaches. The technology will facilitate the discovery of new, corrosion-resistant materials to improve safety and reduce costs across a variety of industries.

Lawrence Livermore National Laboratory – Livermore, CA

Machine learning Assisted Generation of Next-generation Electronic and Thermodynamic Innovations through Quantum Computing (MAGNETIQC) - $4,107,554

Lawrence Livermore National Lab will develop quantum and machine learning-accelerated software tools and apply them to discovering ultra-strong, lightweight magnets crucial for electric motors and generators and future high-performance information technology. The project technology's core innovation is a highly scalable, hybrid classical-quantum algorithm. Application of this innovation will enable accurate prediction of material performance and rapid development of novel magnetic and spintronic devices.

ColdQuanta, Inc. [d.b.a. Infleqtion] – Boulder, CO

Quantum-Classical Ab Initio Co-Simulation of Unconventional Superconductors (QASUS) - $3,949,109

Infleqtion aims to discover new high-temperature superconductors, materials that conduct electricity with zero losses. Superconductors are used in powerful electromagnets for MRI machines but have found limited use in the electric grid due to the need for ultra-low temperatures. Infleqtion will use their neutral atom quantum computer and a pioneering new algorithm to improve our understanding of superconductivity and discover new, previously unknown, superconductor materials.

Alice & Bob USA, Inc. – Cambridge, MA

Quantum-Accelerated Discovery of Rare-Earth-Free permanent magnets - $3,911,986

Alice & Bob USA will develop and optimize fault-tolerant quantum algorithms that simulate magnetic materials to develop rare-earth-free permanent magnets. These magnets are a key component in many industrial applications, particularly motors and generators. The development of these magnets would bolster U.S. independence from imported critical minerals. The algorithm developed will also be easily adapted to solve other challenging problems in chemistry and materials science. Alice & Bob designs superconducting cat qubits, which are thousands of times more resilient against certain quantum errors.

Lawrence Berkeley National Laboratory – Berkeley, CA

SuperKIQ: Superconductor Search through Krylov-Inspired Quantum Algorithms - $4,449,973

Lawrence Berkeley National Laboratory will combine modern material-design techniques with the capabilities of emerging quantum hardware to deepen our understanding of high-temperature superconductors and accelerate the discovery of new superconducting materials. Superconductors offer loss-free electrical transport, but existing ones require cryogenic conditions and are difficult to form into wires, which limits their applications. This project aims to discover new superconductors by co-designing novel algorithms and quantum error correction protocols for quantum hardware with reconfigurable connectivity.

Xanadu Quantum Technologies, Inc. – Seattle, WA

Quantum Computing Platform for Next-Generation Batteries - $2,027,507

Xanadu Quantum Technologies aims to develop quantum algorithms that simulate x-ray absorption spectroscopy (XAS), achieving a 100x speedup over classical methods. XAS is a widely used materials characterization technique. Xanadu will work with battery experts to use quantum simulations to analyze the XAS data to understand defects as they develop inside fully assembled batteries, enabling development of safer and longer-lasting batteries.

Quantinuum, LLC – Broomfield, CO

Quantum Computing for Modeling Nuclear Quantum Effects in PEM Fuel Cells and Electrolyzers - $4,097,637

Quantinuum will develop quantum algorithms optimized for its trapped ion quantum computer hardware. These algorithms will target dynamical simulations of proton exchange membranes (PEM) and electrocatalysts for improved hydrogen fuel cells and electrolyzers. These devices could enable production of low-cost hydrogen as a fuel and chemical feedstock. The quantum simulations developed for this effort will be useful across the energy sector and applicable to a wide range of chemical reactions, such as fossil fuel processing.

Phasecraft, Inc. – Washington, DC

Quantum Computing for Hydrogen Fuel Production - $4,519,658

Phasecraft Inc. will utilize machine learning and develop highly optimized quantum algorithms for simulating electrolysis, the process of using electric currents to drive chemical reactions. The project's primary objective is to reduce the current reliance on critical minerals, specifically iridium, in electrolysis processes. This effort will initially focus on enhancing low-cost hydrogen production but is anticipated to yield insights applicable to a variety of industrial sectors, including electroplating and metallurgy.

California Institute of Technology – Pasadena, CA

Quantum Algorithms for Accelerated Discovery of Bioelectrocatalytic Materials for Nitrogen Fixation - $3,765,866

California Institute of Technology will develop a novel bio-electrocatalyst to significantly reduce the energy requirements for ammonia production. Ammonia is a key component of modern fertilizers, the production of which accounts for up to 1/3 of total agricultural energy use. It is possible to reduce the energy footprint of ammonia production by utilizing biological pathways coupled with electrochemical driving forces derived from alternative sources. Caltech will develop quantum algorithms that provide a 1000x speedup, removing a key bottleneck in discovering new catalysts to accelerate and economize this important industry.

PsiQuantum, Corp. – Palo Alto, CA

Quantum-Enabled Direct Methane-to-Methanol (DMTM) - $3,641,923

PsiQuantum will develop fault-tolerant quantum computing workflows integrating quantum chemistry simulations, classical computation, and high-throughput experiments to design new catalysts for direct conversion of methane to methanol. Through utility-scale quantum computing, these workflows aim to ultimately convert methane (natural gas, which is often vented or flared) into methanol, a valuable chemical feedstock and energy-dense liquid fuel that is easier to store, distribute, and use in the transportation sector.