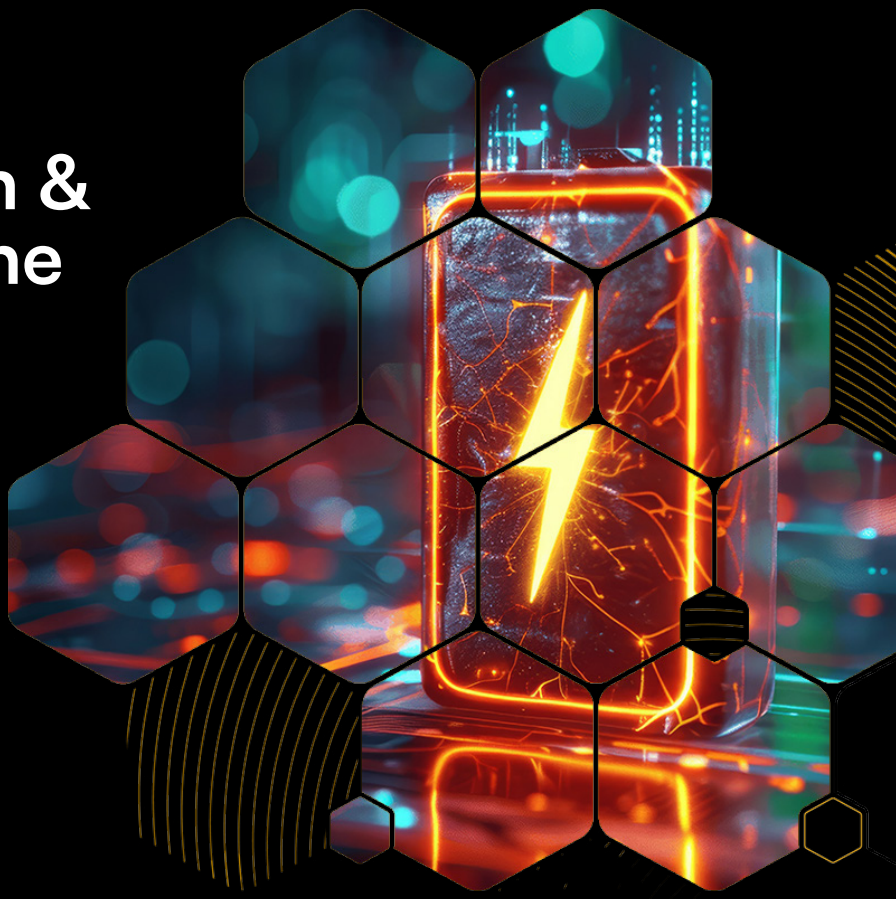
SANDBOXAQ

AQVolt: Simulation & Optimization for the Battery Industry



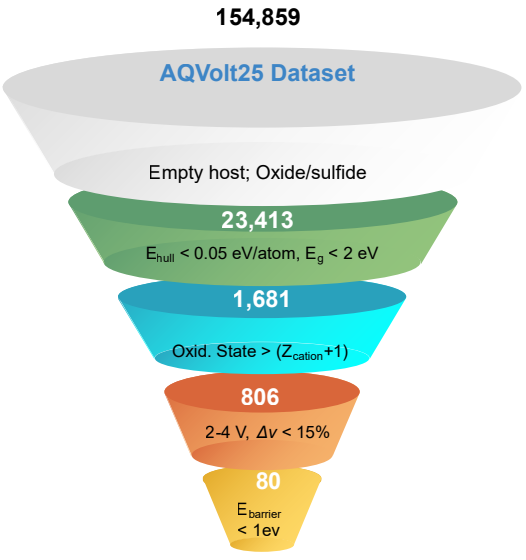
Better, Cheaper, Faster Battery R&D

Designing, optimizing, and manufacturing new battery materials is slow and expensive. Worse, R&D and testing failures can haunt manufacturers once products go to market. SandboxAQ revolutionizes battery R&D, cutting development timelines from years to days.

How Does It Work?

No quantum computer needed. SandboxAQ's cloud-native software runs on classical hardware, combining the accuracy of quantum mechanical predictions with the speed of AI-driven insights. SandboxAQ has developed software that can solve these battery design and production problems repeatedly and at scale. Using quantitative AI and physics-based techniques, our **AQVolt platform** helps you bring new products to market, faster, cheaper, and with more confidence than ever before by generating our own data to build **Large Quantitative Models** (LQMs).

Validated Discovery of 3 New Cobalt-Free Battery Cathode Materials



3 candidates
($FeMoClO_4$, VP_2O_7, $FePO_4$)

Quantitative AI for Battery Materials Use Cases

Our proprietary data generation workflows in AQVolt combine active learning, enhanced sampling techniques, and automated pipelines. We generate diverse and chemically rich datasets tailored to each use case, powering specialized ML force fields (MLFFs) that retain quantum mechanical accuracy at massive scale. Our approach ensures high extrapolation performance across wide chemical spaces. For AQVolt25, we generated thousands of high-fidelity samples with the Google Cloud Platform and trained machine learning interatomic potentials that enable chemically accurate simulations novel battery materials, orders of magnitude faster than traditional methods. These simulations are critical to expediting the identification of next-generation solid-state electrolytes for Novonix, U.S. Army C5ISR, and our other partners.

DESIGN OF COBALT-FREE CATHODE MATERIALS

- Rapidly identify lithium intercalation sites and diffusion pathways across candidate structures.
- Screen compositions for structural integrity during lithiation—quantify volume change, thermodynamic stability, and conversion risk.

DISCOVERY OF SOLID-STATE ELECTROLYTES

- Predict ionic conductivity and activation barriers via MLFF-accelerated MD simulations.
- Filter candidates based on diffusion properties, electrochemical stability windows, and electrode compatibility.
- Deliver ranked SSE formulations optimized for conductivity, stability, and practical processing.

What Can We Do For You?

SandboxAQ's AQVolt platform is adaptable, collaborative, and easy to use. Customers throughout the battery industry can leverage our solutions to supercharge innovation.

To learn more, please talk to one of our experts today and visit us at sandbox.com.

PREDICT

Predict chemical & physical properties with unmatched confidence, through a unique DFT + ML-based hybrid model and powerful AI-driven insights.

DISCOVER

Accelerate chemistry & materials discovery with efficient high-throughput virtual screening and physics-derived synthetic data to predict emergent properties.

OPTIMIZE

Optimize cell design, material chemistries, electrolyte formulations, and electrode coatings using advanced surrogate ML models.

Contact Us Today

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