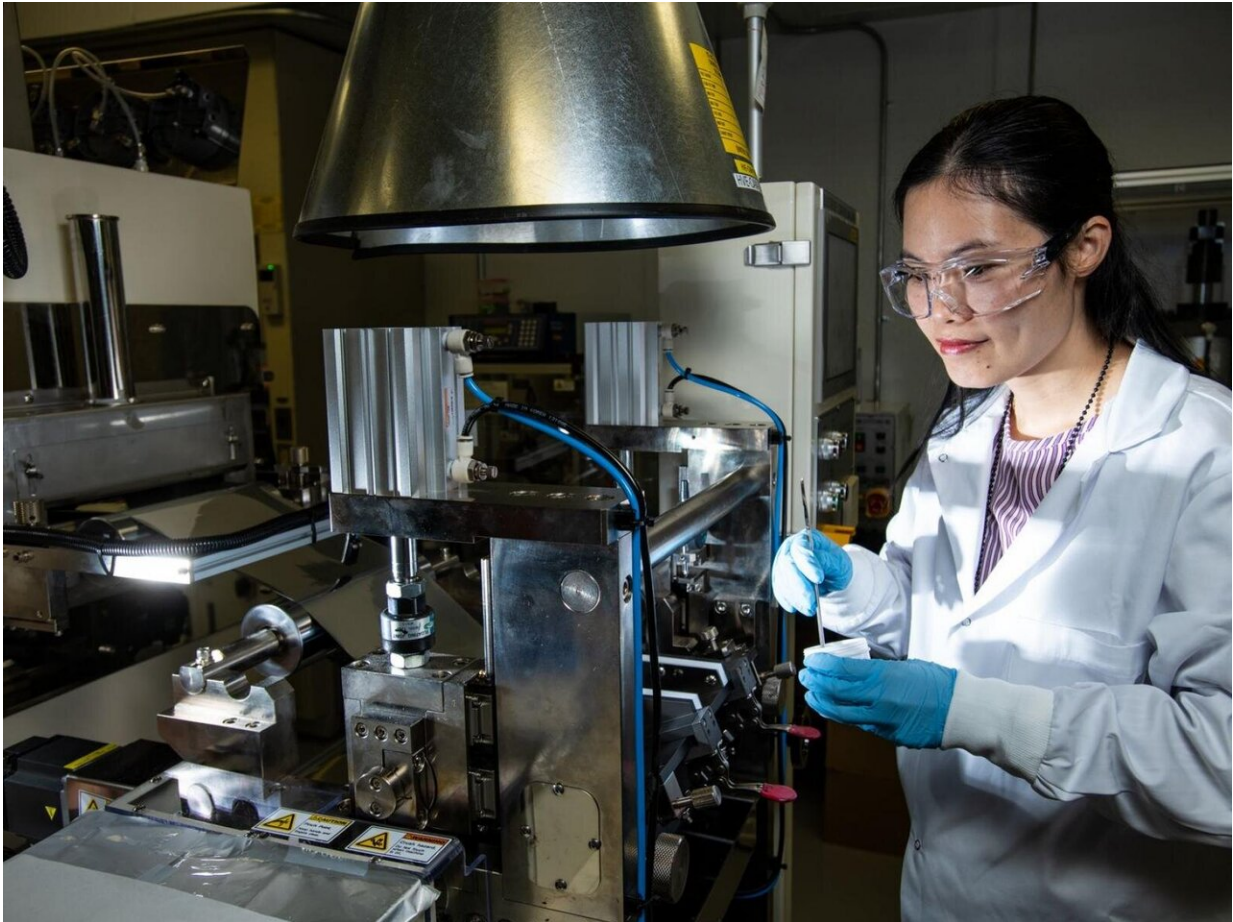# Building a better battery, faster

July 10 2020, by Susan Bauer

PNNL battery researchers and computer experts have created a battery design app. Credit: Andrea Starr | PNNL

Battery experts at PNNL and elsewhere focus on developing rechargeable lithium-metal batteries because of their high energy

density. Lithium-metal batteries have the potential to double the energy of lithium-ion batteries commonly used today in electric vehicles and cell phones. But the right combination of component materials and design is tricky.

Now, PNNL has developed a [software tool](#) that helps universities, [small business](#), and corporate developers to design better batteries with new materials that hold more energy.

Machine Learning is key to battery design recommendations

Dubbed Li-Batt Design App, the [software](#) uses [machine learning](#) to provide the design answers needed. Unlike commercial lithium-ion batteries, the cell design of these batteries—in which the negative electrode is made of up lithium-metal—is very different.

Because there are so many potential cathode materials, finding the right combination and configuration quickly is a challenge. So PNNL battery experts and computational gurus developed a first-of-its-kind software to help battery researchers and commercial developers rapidly design lithium-metal pouch cells. Pouch cells are prototypes of battery cells similar to a [cell phone](#)-sized battery. With the software, the size of the pouch cells is adjustable to meet different applications.

PNNL leads the U.S. Department of Energy's Battery 500 Consortium, which aims to significantly improve battery technology that powers electric vehicles. It's focused on developing commercially viable electric vehicle batteries with cell level specific energies of 500 Wh/kg. Through the consortium, researchers gathered enough experimental data on high energy lithium-metal batteries to "train" the machine learning engine that runs the software.

Li-Batt Design App's trained software helps users custom design a lithium-metal battery based on currently available lithium-metal anodes or even "anode free," cathodes and cell accessories. The simple, flexible interface also enables developers to input any new cathode material developed by the users along with information on the voltage and capacity needed. The software generates a mathematical solution based on design parameters. The researchers can immediately make a prototype lithium-metal battery by using the suggested parameters exported from the software.

Design software available for researchers and commercial developers

Li-Batt Design App is available under a simple, standard site license agreement, and several universities, small businesses, and multi-national companies have already begun using it. Researchers at PNNL are interested in collaborating with teams working on lithium-metal battery development. PNNL is currently developing additional software, which complements the Li-Batt Design App, to assist with design of lithium-metal batteries in form factors and configurations relevant to grid applications, electric vehicles, and many kinds of small electronic devices.

More information: Li-Batt Design App: www.pnnl.gov/technology/li-batt-design-app

Provided by Pacific Northwest National Laboratory

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