Nano Focus

"Ada" demonstrates capabilities of a self-driving laboratory

Ada is a robotic laboratory that discovers and develops new organic thin-film materials without any human supervision. Its productivity will put most graduate students to shame. The entire thin-film fabrication cycle—from the mixing of chemical precursors, deposition, and thermal anneal, to the final electrical and optical characterization—takes only 20 minutes. Ada took only 30 hours to discover the optimum chemical composition of a new hole transport material used in organic solar cells, as reported by a Canadian research team in a recent issue of *Science Advances* (doi:10.1126/sciadv.aaz8867).

Thin-film devices often show interesting thermal, electrical, and optical properties that find applications as sensors and actuators. Photovoltaic cells are typically made of many layers of thin films stacked on top of each other. The properties of these films are highly sensitive to material parameters such as thickness, morphology, and defect chemistry, which are in turn affected by processing parameters such as dopant concentration, number of layers, annealing time and temperature, and substrate type, for example. The large parameter space available for experimentation makes a thin-film system a challenging optimization problem.

For this specific study, Ada was tasked with discovering the optimum concentration of cobalt in spiro-OMeTAD, a material used to conduct charges in a solar cell. The experimentation begins when a robotic arm turns the cap of a chemical vial, draws out the required volume using a pipette, and drops the solution on a glass slide. A spin coater spreads the solution into a thin film, which is then baked in a stream of hot air. Repetitions of this experiment iterate over different cobalt concentrations and annealing times. "Dopant ratio is one of the most frequently manipulated compositional variables when optimizing device performance, and thermal annealing is among the most commonly manipulated processing variables," the researchers, led by A. Aspuru-Guzik of the University of Toronto, and J.E. Hein and C.P. Berlinguette of The University of British Columbia, told *MRS Bulletin*.

The robotic laboratory Ada is named after Ada Lovelace, one of the pioneers of computer programming. Credit: Fraser Parlane, Berlinguette Group, The University of British Columbia.

Ada characterizes each film using in-built systems for dark-field photography, ultraviolet–visible–near-infrared (UV-vis-NIR) reflection and transmission spectroscopy, and four-point probe conductance measurement. These measurements are fed into ChemOs—the internal software that runs Ada—which then suggests the parameters for the next round of experiments using a Global Bayesian Optimization Algorithm. "ChemOS created a surrogate model of the experimental response surface, and updated this model with each round of data that the platform obtained," said the researchers.

In 35 cycles, Ada determined that the best performing spiro-OMeTAD thin films have 0.4 equivalents of cobalt and are not to be annealed for more than 75 seconds. Future experiments will explore a larger parameter space by introducing other variables into the optimization process. "We made the strategic decision to confine it to a smaller number of parameters to illustrate the concept," the researchers explained.

Ada joins a number of recent robotic laboratories that are propelling high-throughput experimental investigations in materials systems as varied as carbon nanotubes, amorphous alloys, and perovskite quantum dots. "Materials discovery and design can be substantially accelerated through AI [artificial intelligence]-driven, high-throughput methods. This work demonstrates these ideas, building a remarkably modular and reproducible system, enabling adoption by both academia and industry, and consequently shortening the research and development time for novel materials across the application spectrum," said James Warren, director of the Materials Genome Program at the National Institute of Standards and Technology.

His views were echoed by Kristofer Reyes at the University at Buffalo, The State University of New York: "This is exciting work that shows how even complex, multistep preparation, synthesis, and characterization—along with ML [machine learning]-assisted decision-making and planning—can all be done in one, autonomous system. It really helps clarify the prospect and potential of even more complex 'all-in-one,' self-driving labs."

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