‘Self-Driving’ Lab Speeds Up Research, Synthesis of Energy Materials

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Researchers from North Carolina State University and the University at Buffalo have developed and demonstrated a ‘self-driving lab’ that uses artificial intelligence (AI) and fluidic systems to advance our understanding of metal halide perovskite (MHP) nanocrystals. This self-driving lab can also be used to investigate a broad array of other semiconductor and metallic nanomaterials.

“We’ve created a self-driving laboratory that can be used to advance both fundamental nanoscience and applied engineering,” says Milad Abolhasani, corresponding author of a paper on the work and an associate professor of chemical and bimolecular engineering at NC State.

For their proof-of-concept demonstrations, the researchers focused on all-inorganic metal halide perovskite (MHP) nanocrystals, cesium lead halide (CsPbX3, X=Cl, Br). MHP nanocrystals are an emerging class of semiconductor materials that, because of their solution-processability and unique size- and composition-tunable properties, are thought to have potential for use in printed photonic devices and energy technologies. For example, MHP nanocrystals are very efficient optically active materials and are under consideration for use in next-generation LEDs. And because they can be made using solution processing, they have the potential to be made in a cost-effective way.

Solution-processed materials are materials that are made using liquid chemical precursors, including high-value materials such as quantum dots, metal/metal oxide nanoparticles and metal organic frameworks.

However, MHP nanocrystals are not in industrial use yet.

“In part, that’s because we’re still developing a better understanding of how to synthesize these nanocrystals in order to engineer all of the properties associated with MHPs,” Abolhasani says. “And, in part, because synthesizing them requires a degree of precision that

has prevented large-scale manufacturing from being cost-effective. Our work here addresses both of those issues."

The new technology expands on the concept of Artificial Chemist 2.0, which Abolhasani's lab unveiled in 2020. Artificial Chemist 2.0 is completely autonomous, and uses AI and automated robotic systems to perform multi-step chemical synthesis and analysis. In practice, that system focused on tuning the bandgap of MHP quantum dots, allowing users to go from requesting a custom quantum dot to completing the relevant R&D and beginning manufacturing in less than an hour.

"Our new self-driving lab technology can autonomously dope MHP nanocrystals, adding manganese atoms into the crystalline lattice of the nanocrystals on demand," Abolhasani says.

Doping the material with varying levels of manganese changes the optical and electronic properties of the nanocrystals and introduces magnetic properties to the material. For example, doping the MHP nanocrystals with manganese can change the wavelength of light emitted from the material.

"This capability gives us even greater control over the properties of the MHP nanocrystals," Abolhasani says. "In essence, the universe of potential colors that can be produced by MHP nanocrystals is now larger. And it's not just color. It offers a much greater range of electronic and magnetic properties."

The new self-driving lab technology also offers a much faster and more efficient means of understanding how to engineer MHP nanocrystals in order to obtain the desired combination of properties.

"Let's say you want to get an in-depth understanding of how manganese-doping and bandgap tuning will affect a specific class of MHP nanocrystals, such as CsPbX3," Abolhasani says. "There are approximately 160 billion possible experiments that you could run, if you wanted to control for every possible variable in each experiment. Using conventional techniques, it would still generally take hundreds or thousands of experiments to learn how those two processes – manganese-doping and bandgap tuning – would affect the properties of the cesium lead halide nanocrystals."

But the new system does all of this autonomously. Specifically, its AI algorithm selects and runs its own experiments. The results from each completed experiment inform which experiment it will run next – and it keeps going until it understands which mechanisms control the MHP's various properties.

"We found, in a practical demonstration, that the system was able to get a thorough understanding of how these processes alter the properties of cesium lead halide nanocrystals in only 60 experiments," Abolhasani says. "In other words, we can get the information we need to engineer a material in hours instead of months."

While the work demonstrated in the paper focuses on MHP nanocrystals, the autonomous system could also be used to characterize other nanomaterials that are made using solution processes, including a wide variety of metallic and semiconductor nanomaterials.

"We're excited about how this technology will broaden our understanding of how to control the properties of these materials, but it's worth noting that this system can also be used for continuous manufacturing," Abolhasani says. "So you can use the system to identify the best possible process for creating your desired nanocrystals, and then set the system to start producing material nonstop – and with incredible specificity.

"We've created a powerful technology. And we're now looking for partners to help us apply this technology to specific challenges in the industrial sector."

The paper, "Autonomous Nanocrystal Doping by Self-Driving Fluidic Micro-Processors," is published open access in the journal Advanced Intelligent Systems. The paper was co-authored by Fazel Bateni, a Ph.D. student at NC State; Robert Epps and Jeffery Bennett, postdoctoral researchers at NC State; Kameel Antami, a former Ph.D. student at NC State; Rokas Dargis, an undergraduate at NC State; and Kristofer Reyes, an assistant professor at the University at Buffalo.

Read the original article on North Carolina State University.