'Natural selection' could lead to amazing new materials

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Teflon and Kevlar are man-made materials that have changed the world. They were also invented by accident.

Colorado State University scientists want to take the guesswork out of making the next world-changing material. They're embarking on a brave new world of materials discovery, supported by a W.M. Keck Foundation research grant.

Amy Prieto and Jamie Neilson, both faculty members in the Department of Chemistry, have been jointly awarded $1 million from the Keck Foundation to develop a novel method for discovering new, functional materials. Their goal: to perfect a process to precisely engineer materials exhibiting specific, desirable properties – be that tensile strength, heat resistance, or conductivity, to name a few – rather than using traditional processes of trial and error, or relying on incomplete theory to predict new structures.

"The normal way to find a new material is to make a lot of new materials, screen them, and hope you get lucky," Prieto said. "There are no guiding principles for how to strategically only make one material with the properties that you want."

aid Neilson: "We're flipping the problem upside down. Rather than thinking linearly, we're asking, what property do we want? Let's design a way to make a new material that will only work if it has the property that we are interested in."

Take the materials in a battery. Prieto has a start-up company, Prieto Battery, working on next-generation materials for better, non-toxic batteries. What's the bottleneck? The materials in a battery are inherently "messy," Prieto says. They can't be modeled accurately yet, because the ions in the electrolyte are constantly moving, and battery structure often contains, or even relies on defects to work properly. Their new method could accelerate the development of new materials for sodium or magnesium-based batteries, in which needed materials are 20 years away, the Keck proposal asserts.

Natural selection for materials

So what will this new process look like? The researchers propose a setup that uses a well-known ion-conducting material, silver iodide, as a test case to prove their principle. And what better way than to take cues from nature? They're calling their method "natural selection" for materials. Instead of starting with a known compound and trying to optimize its properties, they will use fundamental physical properties required for a specific application to guide and select for the synthetic conditions, and the resulting materials. That way, only those materials that behave in the desired way will form.

Once they've made their material, they then need to figure out what they made. Part of their research grant, which is furthered bolstered by university support, involves new instrumentation to precisely characterize materials.

One of the new pieces of equipment is an X-ray diffractometer, which scatters X-rays off the surface of the material to create a pattern of visual information about the material's atomic structure. The other is a sample holder for an existing transmission electron microscope, a powerful imaging tool that uses an electron beam, as opposed to light, to let researchers watch atomic-level changes in materials as they grow.

These new instruments are critical to their three-year Keck project, which will include the naming of a new Keck Center for Materials Discovery.

James Sites, associate dean of the College of Natural Sciences, points to the two-fold importance of Neilson and Prieto's work: "They are blazing a new path not only in materials discovery, but also, in inspiring the next generation of materials scientists. They are very deserving of this incredible honor from the Keck Foundation."

Provided by Colorado State University

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