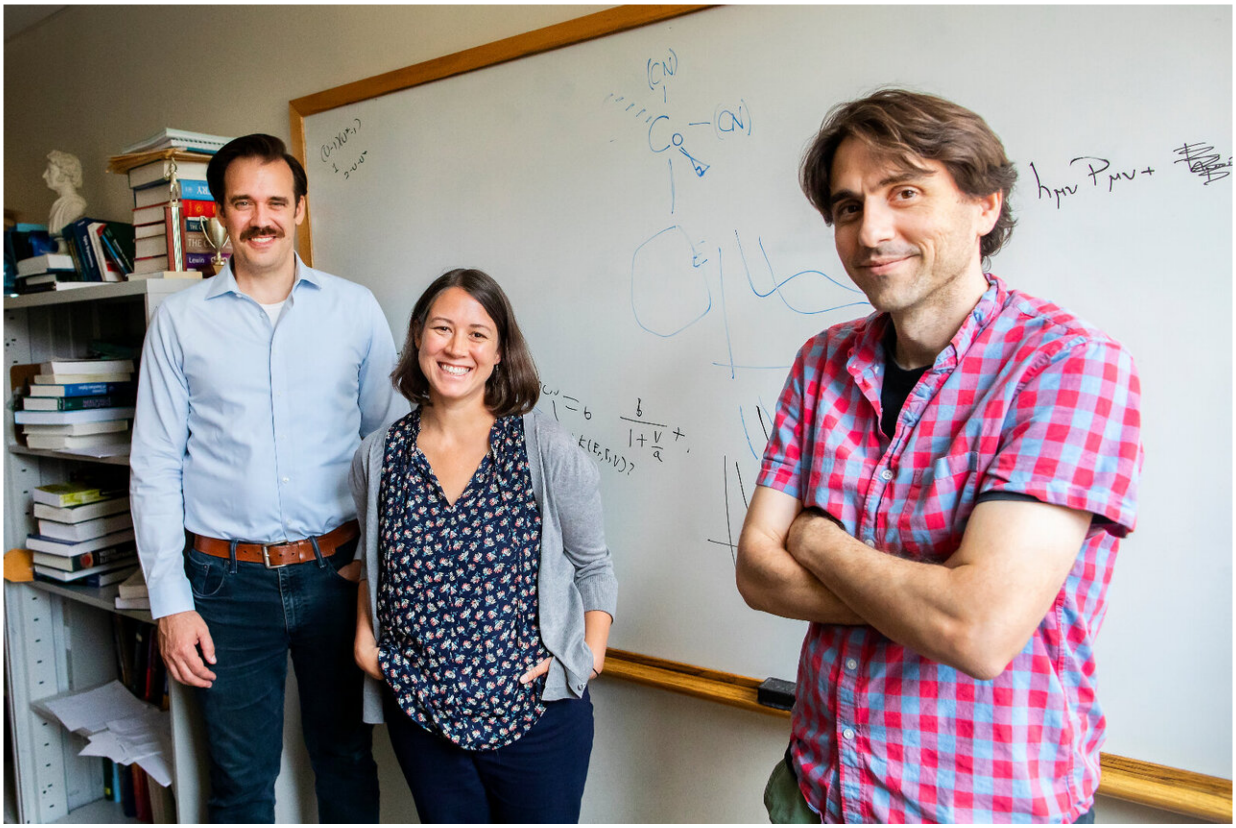
Unlocking the power of a molecule's spin

February 1 2021, by Erica K. Brockmeier



A new study led by Joseph Subotnik (right) describes a theoretical framework that could allow experimentalists to have better control over chemical reactions by using a molecule's spin. Using this framework, future experiments conducted through the Center for Sustainable Separations of Metals (CSSM) with Eric Schelter (far left) and Jessica Anna could help researchers develop more energy-efficient ways to purify and recycle scarce materials such as rare earth metals (pre-pandemic image). Credit: University of Pennsylvania

Behind the devices that shape modern life is an array of natural and human-made materials. One such component of smartphones and computers are rare earth metals, a group of 17 elements that, because they aren't found in concentrated deposits, require energy-intensive and toxic methods to extract. While recycling rare earth metals from used devices is one way to relieve strained supply chains and reduce environmental damage, the fundamental chemistry required for efficiently separating and reusing these metals remains a challenge.

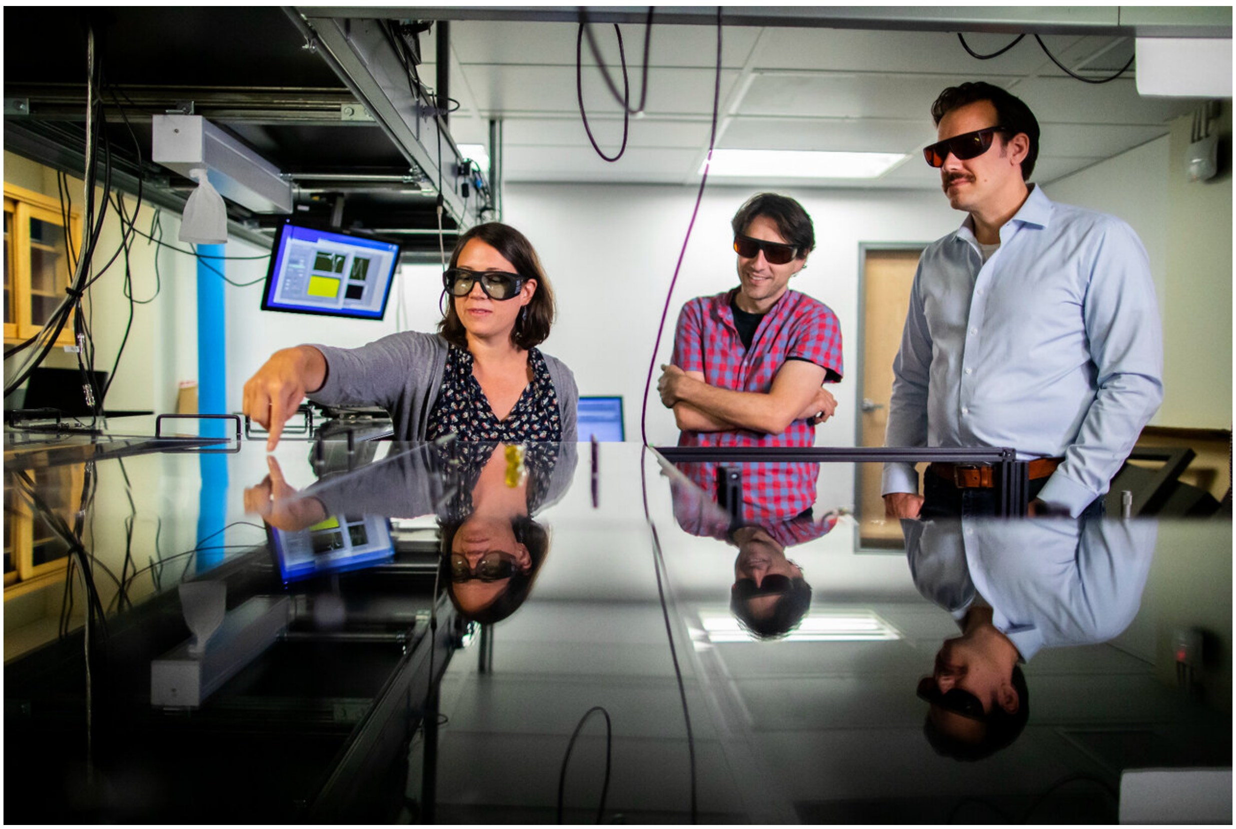
Now, new research provides a theoretical framework that could change the paradigm for how chemicals are separated. Graduate student Yanze Wu and professor Joseph Subotnik describe in *Nature Communications* how a molecule's spin can be used to control a chemical reaction. Based on this concept, future experiments conducted through the Center for Sustainable Separations of Metals (CSSM) could help researchers develop more energy-efficient ways to purify and recycle scarce materials such as rare earth metals.

The goal of the CSSM, established in 2019 and led by a team of Penn chemists, is to develop chemical separation methods that make the process of recycling metals from consumer products more cost-effective. CSSM brings together theoretical and experimental chemistry groups, with the goal of conducting fundamental research that provides creative, scientifically-driven solutions to the rare earth metal supply chain crisis.

Subotnik, a theoretical chemist, had previously been working on questions related to photochemistry and was interested in understanding how light impacts molecules. In the process of trying to better understand the dynamics of photochemical reactions, he and Wu began to postulate the role of spin during light-induced changes to a molecule's energy state. After spending a year delving deeply into this area of study, Subotnik realized through conversations with CSSM Director Eric

Schelter that this theoretical work could also have implications for metal separation.

"One of the reasons rare earth metal separation is hard is because a lot of metals are very similar to each other. But one of the properties of a metal is that it has certain spin properties," Subotnik says. "One idea is that if you want to separate metals, you might be able to use spin properties, which can be very different."



To help validate their findings, Subotnik will be working with Schelter and Anna to conduct follow-up experiments and combine those data with new theoretical models (pre-pandemic image). Credit: University of Pennsylvania

In this new theoretical framework, the researchers show that spin helps molecules as they pass through unstable geometries during a chemical reaction. Subotnik uses the analogy of finding a secret mountain pass and how controlling spin could enable someone to travel to a specific place, in this case a particular product of a chemical reaction, on the other side. "We show that a little bit of spin can force you to take one pass versus the other with a huge fidelity, and just a little bit of spin can guide which product you're going to make," he says.

What's significant about this idea is that a molecule's spin can be changed using a very small amounts of energy, and this small change in spin also has enormous effects on how a chemical reaction proceeds. While using spin to power devices has been the ambition of fields like spintronics, its implications in fundamental chemistry have not been widely explored. "The question is, Can you use these really small energies to make nonintuitive chemistry happen," says Subotnik. "If I understand spin and can manipulate it, could I promote one reaction or the other, to get one metal to separate rather than another?"

But what makes this discovery exciting also makes the next steps challenging: "It's powerful, but it's hard to diagnose," Subotnik says. Because a molecule's spin rotates with the molecule itself and averages out during experiments, it's difficult to isolate spin's impacts in lab measurements. To help validate their findings, Subotnik will be working with Schelter and Jessica Anna to conduct follow-up experiments and combine those data with new theoretical models.

"The recent announcements by the Biden administration and General Motors for a wholesale shift to electric vehicles will create huge demands for mining lithium, cobalt, rare earths, and other critical metals," says Schelter, "Joe and Yanze's work has important implications for fundamentally new and selective separations of critical metals that could reduce energy consumption, waste, and greenhouse gas production associated with mining, or enable critical metals recycling."

Beyond its implications for metal separation, this framework also paves the way for a new paradigm on how electrical, spin, and other chemical properties could be combined in ways that have not been explored before. "Nobody's really combined these aspects of spin and chemistry before, so I do''t know what's going to happen," Subotnik says. "The dream would be that you make some process way more efficient. That's fundamental science at its best."

More information: Yanze Wu et al. Electronic spin separation induced by nuclear motion near conical intersections, *Nature Communications* (2021). DOI: 10.1038/s41467-020-20831-8

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