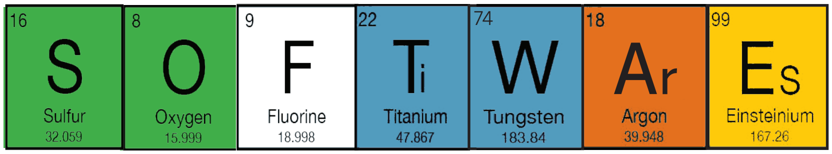

C H E M I S T R Y

Professor speeds new chemistry for earth-friendly materials

Years of trial and error have made it clear that satisfying consumer needs while safeguarding the environment or lowering energy costs requires a delicate chemistry.

James Chelikowsky had a better idea: let a supercomputer find the right mix of chemicals.

In 2012 ICES Professor Chelikowsky received $6.2 million from the U.S. Department of Energy to help discover materials for low-cost energy applications. Two years later he received $1.2 million from the National Science Foundation to help discover materials to improve magnets.

A professor of physics, chemistry, and chemical engineering, Chelikowsky actually develops software, not materials. But his high-dollar software skills, now 20 years under development, allow him to slog through near-infinite complex chemical combinations, and determine their suitability for the task at hand.

"The software we develop helps eliminate the expensive trial and error of laboratory experiments trying to predict and understand the properties of materials," said Chelikowsky, who won the American Physical Society's highest award in the field of computational physics: the Aneesur Rahman Prize for Computational Physics.

"Our new code will incorporate, and thus shortcut for other researchers, the enormously complex equations that predict properties of materials solely from knowledge of their chemical composition," he said.

Low-cost Energy

Potential uses for new energy materials include economical battery materials to capture solar energy and materials that convert water to hydrogen using sunlight.

The wide range of materials problems associated with energy-related applications requires a team of physical scientists, materials engineers, computer scientists and applied mathematicians. This diverse research team will develop and implement scalable, open-source codes to be used across the scientific community, he said.

"We already know that the physical basis for predicting properties of materials exists within the quantum mechanical theory of atoms," said Chelikowsky, director of the ICES Center for Computational Materials. "Our team's software will aid in the design of new materials and efficiently ascertain a material's viability for energy applications.

"In the end, our software will be open to all," said Chelikowsky. "It should significantly accelerate the discovery of new materials for energy applications."

Environmentally Friendly Magnets

Magnets drive electric motors, encode data on computer hard drives, and enable MRI machines to image the insides of bodies.

But the powerful, permanent magnetics in most high-tech products are not the same magnets stuck on your fridge. They contain rare-earth metals, which help boost magnetic strength to about 250 times that of the front-of-the-refrigerator variety.

On a global distribution scale, these metals are not all that rare. (Neodymium, the most widely used rare-earth, is about as common in the earth's crust as copper.) However, their continued accessibility and potential environmental effects are a reason for concern: China produces 97 percent of all rare-earths, and the rare-earth mining process can release dangerous radioactive elements, such as uranium, into the environment.

To ensure access to powerful magnets, and to make technology more environmentally friendly, we need a way to make magnets strong without resorting to rare-earths, says Chelikowsky. With support from the Natioal Science Foundation he is working to identify the next generation of powerful magnetic materials by computationally analyzing compounds that could offer the same properties as rare-earth magnets without containing any rare-earths themselves.

His work is conducted in collaboration with Iowa State University computational materials researchers Kai-Ming Ho and Cai-Zhuang Wang.

Two Codes Combined

Scientists estimate millions of possible magnetic compounds have yet to be explored—and that's just materials made up of three to four elements.

Prof. Chelikowsky's supercomputer code evaluates the suitability of chemical combinations to be used for energy or magnets.

Chelikowsky and his collaborators are investigating such tertiary and quaternary compounds for exceptional magnetic properties by applying two computer codes with complimentary properties. One code, called the genetic algorithm developed by his Iowa State collaborators, generates compound variations. The other, called PARSEC, analyzes their electronic structure for signs that could indicate good magnetic properties.

PARSEC Advantage

PARSEC (an acronym for pseudopotential algorithm for real-space electronic calculations) is a code that Chelikowsky and his collaborators have been developing for over 20 years to evaluate chemical compounds on high performance computing systems.

"It's efficient because it's one of the few codes that was written specifically for computing many types of materials on state-of-the-art computers."

Using PARSEC to comb through the Genetic Algorithms results will hopefully identify some promising magnetic materials. But learning more about the connection between electron structure and chemical property is a benefit for material science as a whole, said Chelikowsky.

"That's one of the strengths of what we do," Chelikowsky said. "The things that we learn about examining magnetic materials should have implications when examining different types of materials, anything from, complex organic materials, to hard materials like semiconductors, insulators, and dielectrics, with a wide variety of properties."

Back to the Lab

The computational power of PARSEC and the Genetic Algorithm will together identify candidate materials. But the research still requires a traditional chemistry lab to test them. To do that, University of Nebraska professor Dave Sellmyer is synthesizing and analyzing the most promising of the computational predictions to see how they hold up outside of the computational realm.

"We need an experimentalist, for verification and validation. So, we scoured the field to find a superb experimentalist to work with us," Chelikowsky said.

By the end of the grant, the goal is to have identified and synthesized powerful magnets without rare-earths, Chelikowsky said. However, the process of the research, which will include compiling an open access database of magnetic materials and their properties, will likely be valuable in and of itself.

"At the minimum, we'll have a great improvement in magnetic materials, how we look at them, and calculate their properties," Chelikowsky said, "And in the best scenario, we will not only get that, but we will also get the ability to predict new materials and to have actually made new materials."