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Many Bodies, Many Possibilities

How can one predict a material's behavior on the molecular and atomic levels, at the shortest timescales? What's the best way to design materials to make use of their quantum properties for electronics and information science?

These broad, difficult questions are the type of inquiries that UC Santa Barbara theorist Vojtech Vlcek and his lab will investigate as part of a select group of scientists chosen by the U.S. Department of Energy (DOE) to develop new operating frameworks for some of the world's most powerful computers. Vlcek will be leading one of five DOE-funded projects — to the tune of $28 million overall — that "will focus on computational methods, algorithms and software to further chemical and materials research, specifically for simulating quantum phenomena and chemical reactions."

"It's really exciting," said Vlcek, an assistant professor in the Department of Chemistry and Biochemistry, and one of, if not the youngest researcher to lead such a major endeavor. "We believe we will be for the first time able to not only really describe realistic systems, but also provide this whole framework for ultrafast and driven phenomena that will actually set the scene for future developments."

"I congratulate Vojtech Vlcek on being selected for this prestigious grant," said Pierre Wiltzius, dean of mathematical, physical and life sciences at UC Santa Barbara. "It's especially impressive and unusual for an assistant professor to lead this type of complex, multi-institution research project. Vojtech is in a league of his own, and I look forward to future insights that will come from the team's

discoveries.”

A Multilayer Framework

As part of the DOE’s efforts toward clean energy technologies, scientists across the nation study matter and energy at their most fundamental levels. The goal is to design and discover new materials and processes that can generate, manipulate and store energy — techniques that have applications in a wide variety of areas, including energy, environment and national security.

Uncovering these potentially beneficial phenomena and connecting them to the atoms they come from is hard work — work that could be assisted with the use of the supercomputers that are housed in the DOE’s national laboratories.

“DOE’s national labs are home to some of the world’s fastest supercomputers, and with more advanced software programs we can fully harness the power of these supercomputers to make breakthrough discoveries and solve the world’s hardest to crack problems,” said U.S. Secretary of Energy Jennifer M. Granholm. “These investments will help sustain U.S. leadership in science, accelerate basic energy and advance solutions to the nation’s clean energy priorities.”

Among the challenges Vlcek and team will face is the issue of many interacting particles. Interactions are more easily predicted in a system of a few atoms or molecules, or in very regular, periodic systems. But add more bodies or use more elaborate systems and the complexity skyrockets because the characteristics and behaviors of and interactions between every particle have to be accounted for. In some cases, their collective behaviors can produce interesting phenomena that can’t be predicted from the behavior of individual particles.

“People have been working with small molecules, or characterizing perfectly periodic systems, or looking at just a few atoms,” Vlcek said, and more or less extending their dynamics to try to approximate the behaviors of larger, more complex systems.

“This is not necessarily realistic,” he continued. “We want to simulate surfaces. We want to simulate systems that have large-scale periodicity. And in these cases you need to consider systems that are not on nanometer scales, but on the scale of thousands of atoms.”

Add to that complexity non-equilibrium processes, which are the focus of Vlcek's particular project. He will be leading an effort that involves an additional seven co-principal investigators from UC Berkeley, UCLA, Rutgers University, University of Michigan and Lawrence Berkeley National Laboratory.

"Essentially these systems are driven by some strong external stimuli, like from lasers or other driving fields," he said. "These processes are relevant for many applications, such as electronics and quantum information sciences."

The goal, according to Vlcek, is to develop algorithms and software based on "a multilayer framework with successive layers of embedding theories to capture non-equilibrium dynamics." The team, in partnership with two DOE-supported Scientific Discovery through Advanced Computing (SciDAC) Institutes at Lawrence Berkeley and Argonne National Laboratories, begins with the most fundamental assumptions of quantum theory. That foundation is followed by layers that incorporate novel numerical techniques and neural network approaches to take advantage of the intensive computing the supercomputers can perform.

"We still stay with the first principles approach, but we're making successive levels of approximations," Vlcek explained. "And with this approach we'll be able to treat extremely large systems." Among the many advantages of the methodology will be the ability — for the first time — to describe experimental systems in real-time, as they are driven by external forces.

The outcome of the project will be "bigger than the sum of its parts," said Vlcek. Not only will it provide a method of studying and designing a wide variety of present and future novel materials, the algorithms are also meant for future supercomputers.

"One interesting outcome will be that we will also try to connect to future computational platforms, which could possibly be quantum computers," he said. "So this framework will actually allow future research on present and future novel materials as well as new theoretical research."

About UC Santa Barbara

The University of California, Santa Barbara is a leading research institution that also provides a comprehensive liberal arts learning experience. Our academic community of faculty, students, and staff is characterized by a culture of interdisciplinary

collaboration that is responsive to the needs of our multicultural and global society. All of this takes place within a living and learning environment like no other, as we draw inspiration from the beauty and resources of our extraordinary location at the edge of the Pacific Ocean.