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QUANTUM MECHANICS REVEALS NEW DETAILS OF DEEP EARTH

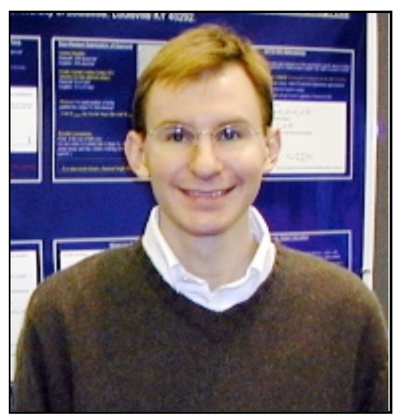
COLUMBUS, Ohio -- Scientists have used quantum mechanics to reveal that the most common mineral on Earth is relatively uncommon deep within the planet.

Using several of the largest supercomputers in the nation, a team of physicists led by Ohio State University has been able to simulate the behavior of silica in a high-temperature, high-pressure form that is particularly difficult to study firsthand in the lab.

The resulting discovery -- reported in this week's early online edition of the *Proceedings of the National Academy of Sciences (PNAS)* -- could eventually benefit science and industry alike.

Silica makes up two-thirds of the Earth's crust, and we use it to form products ranging from glass and ceramics to computer chips and fiber optic cables.

"Silica is all around us," said Ohio State doctoral student Kevin Driver, who led this project for his doctoral thesis. "But we still don't understand everything about it. A better understanding of silica on a quantum-mechanical level would be useful to earth science, and potentially to industry as well."



Kevin Driver

Silica takes many different forms at different temperatures and pressures -- not all of which are easy to study, Driver said.

"As you might imagine, experiments performed at pressures near those of Earth's core can be very challenging. By using highly accurate quantum mechanical simulations, we can offer reliable insight that goes beyond the scope of the laboratory."

Over the past century, seismology and high-pressure laboratory experiments have revealed a great deal about the general structure and composition of the earth. For example, such work has shown that the planet's interior structure exists in three layers called the crust, mantle, and core. The outer two layers -- the mantle and the crust -- are largely made up of silicates, minerals containing silicon and oxygen.

Still, the detailed structure and composition of the deepest parts of the mantle remain unclear. These details are important for geodynamical modeling, which may one day predict complex geological processes such as earthquakes and volcanic eruptions.

Even the role that the simplest silicate -- silica -- plays in Earth's mantle is not well understood.

"Say you're standing on a beach, looking out over the ocean. The sand under your feet is made of quartz, a form of silica containing one silicon atom surrounded by four oxygen atoms. But in millions of years, as the oceanic plate below becomes subducted and sinks beneath the Earth's crust, the structure of the silica changes dramatically," Driver said.

As pressure increases with depth, the silica molecules crowd closer together, and the silicon atoms start coming into contact with oxygen atoms from neighboring molecules. Several structural transitions occur, with low-pressure forms surrounded by four oxygen atoms and higher-pressure forms surrounded by six. With even more pressure, the structure collapses into a very dense form of the mineral, which scientists call alpha-lead oxide.

While these algorithms have been around for over half a century, applying them to silica was impossible until recently, Driver said. The calculations were simply too labor-intensive. Even today, with the advent of more powerful supercomputers and fast algorithms that require less computer memory, the calculations still required using a number of the largest

It's this form of silica that likely resides deep within the earth, in the lower part of the mantle, just above the planet's core, Driver said.

supercomputers in the United States.

When scientists try to interpret seismic signals from that depth, they have no direct way of knowing what form of silica they are dealing with. So they must simulate the behavior of different forms on computer, and then compare the results to the seismic data. The simulations rely on quantum mechanics.

In *PNAS*, Driver, his advisor John Wilkins, and their coauthors describe how they used a quantum mechanical method to design computer algorithms that would simulate the silica structures. When they did, they found that the behavior of the dense, alpha-lead oxide form of silica did not match up with any global seismic signal detected in the lower mantle.

This result indicates that the lower mantle is relatively devoid of silica, except perhaps in localized areas where oceanic plates have subducted, Driver explained.

Wilkins, Ohio Eminent Scholar and professor of physics at Ohio State, cited Driver's determination and resourcefulness in making this study happen. The physicists used a method called quantum Monte Carlo (QMC), which was developed during atomic bomb research in World War II. To earn his doctorate, Driver worked to show that the method could be applied to studying minerals in the planet's deep interior.

"This work demonstrates both the superb contributions a single graduate student can make, and that the quantum Monte Carlo method can compute nearly every property of a mineral over a wide range of pressure and temperatures," Wilkins said. He added that the study will "stimulate a broader use of quantum Monte Carlo worldwide to address vital problems."

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Even today, with the advent of more powerful supercomputers and fast algorithms that require less computer memory, the calculations still required using a number of the largest supercomputers in the United States, including the Ohio Supercomputer Center in Columbus.

"We used the equivalent of six million CPU hours or more, to model four different states of silica" Driver said.

He and his colleagues expect that quantum Monte Carlo will be used more often in materials science in the future, as the next generation of computers goes online.

Coauthors on the paper included Ronald Cohen of the Carnegie Institution of Washington; Zhigang Wu of the Colorado School of Mines; Burkhard Militzer of the University of California, Berkeley; and Pablo López Ríos, Michael Towler, and Richard Needs of the University of Cambridge.

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