Simulations reveal how saltwater behaves in Earth's mantle

June 24 2020, by Emily Ayshford

An artist's depiction of highly compressed saltwater at high temperature. Credit: Zhang et al

Scientists estimate that the Earth's mantle holds as much water as all the oceans on the planet, but understanding how this water behaves is difficult. Water in the mantle exists under high pressure and at elevated temperatures, extreme conditions that are challenging to recreate in the laboratory.

That means many of its physical and chemical properties—relevant to understanding magma production and the Earth's carbon cycle—aren't fully understood. If scientists could better understand these conditions, it would help them better understand the carbon cycle's consequences for climate change.

A team led by Prof. Giulia Galli and Prof. Juan de Pablo from the Pritzker School of Molecular Engineering (PME) at the University of Chicago and Prof. Francois Gygi from the University of California, Davis has created complex computer simulations to better understand the properties of salt in water under mantle conditions.

By coupling simulation techniques developed by the three research groups and using sophisticated codes, the team has created a model of saltwater based on quantum mechanical calculations. Using the model, the researchers discovered key molecular changes relative to ambient conditions that could have implications in understanding the interesting chemistry that lies deep beneath the Earth's surface.

"Our simulations represent the first study of the free energy of salts in water under pressure," Galli said. "That lays the foundation to understand the influence of salt present in water at high pressure and temperature, such as the conditions of the Earth's mantle." The results were published June 16 in the journal *Nature Communications*.

Important in fluid-rock interactions

Understanding the behavior of water in the mantle is challenging—not only because it is difficult to measure its properties experimentally, but because the chemistry of water and saltwater differs at such extreme temperatures and pressures (which include temperatures of up to 1000K and pressures of up to 11 GPa, 100,000 times greater than on the Earth's surface.)

While Galli previously published research on the behavior of water in such conditions, she and her collaborators at the Midwest Integrated Center for Computational Materials (MICCoM) have now extended their simulations to salt in water, managing to predict much more complex properties than previously studied.

The simulations, performed at UChicago's Research Computing Center using optimized codes supported by MICCoM, showed key changes of ion-water and ion-ion interactions at extreme conditions. These ion interactions affect the free energy surface of salt in water.

Specifically, researchers found that dissociation of water that happens due to high pressure and temperature influences how the salt interacts with water and in turn how it is expected to interact with surfaces of rocks at the Earth's surface.

"This is foundational to understanding chemical reactions at the conditions of the Earth's mantle," de Pablo said.

"Next we hope to use the same simulation techniques for a variety of solutions, conditions, and other salts," Gygi said.

More information: Cunzhi Zhang et al, Dissociation of salts in water under pressure, *Nature Communications* (2020). DOI:

10.1038/s41467-020-16704-9

Provided by University of Chicago