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Study unveils new superionic states of helium-water compounds

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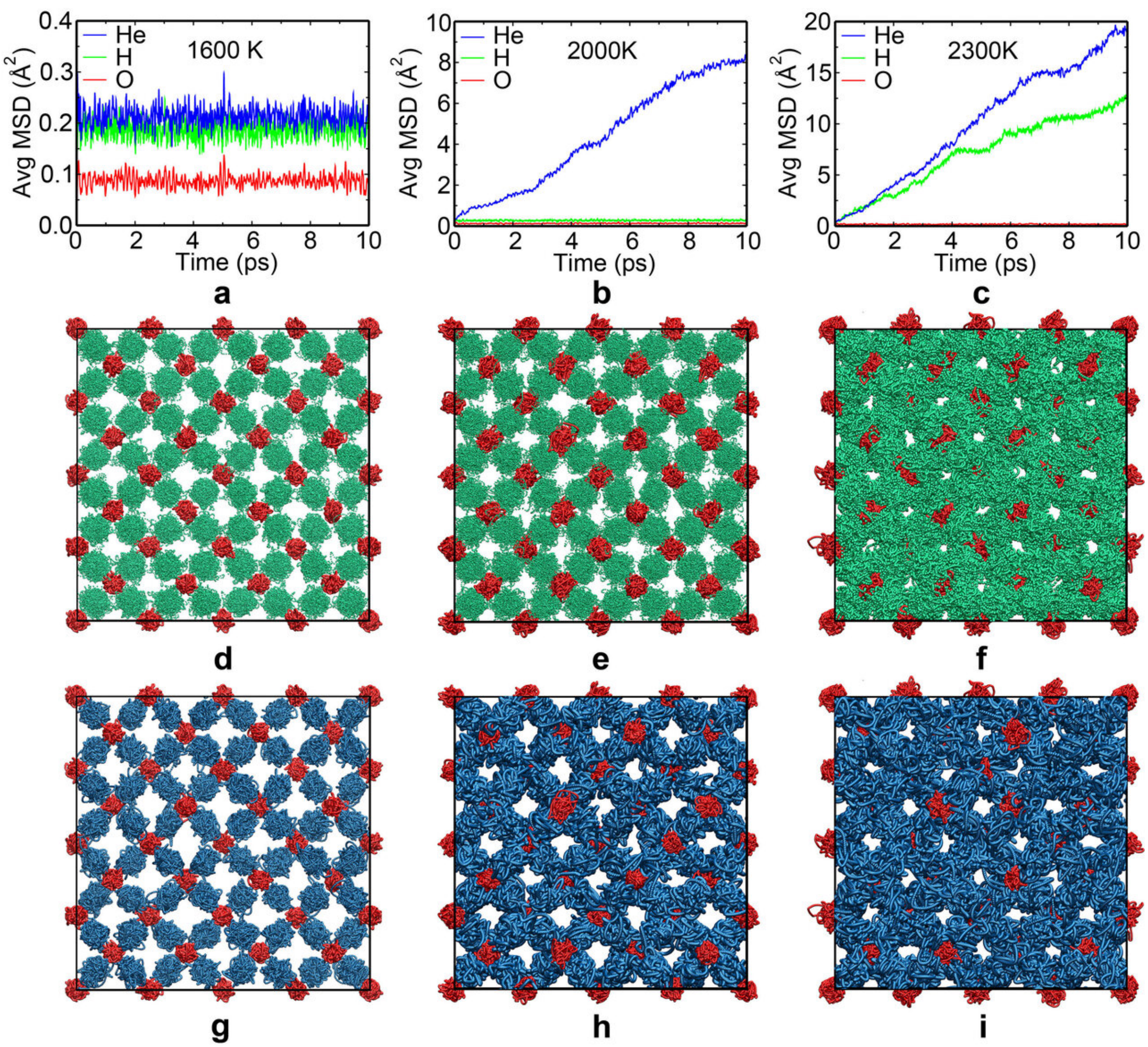


Behaviour of H and He atoms compared to O atoms in Fd-3m He2H2O from AIMD simulations at 1,600 K, 2,000 K and 2,300 K. (a–c) The averaged MSDs for the H, He and O atoms from AIMD simulations at different temperatures. (d–i) Representation of atomic trajectories in one supercell from the simulations from the last 5 ps run representing the three distinct phases: the solid phase (1,600 K), the superionic He phase (2,000 K), SI-I, and superionic He + H phase (2,300 K), SI-II. To avoid overlapping, only H and O are shown in d–f, and only He and O are shown in g–i. Credit: Liu et al.

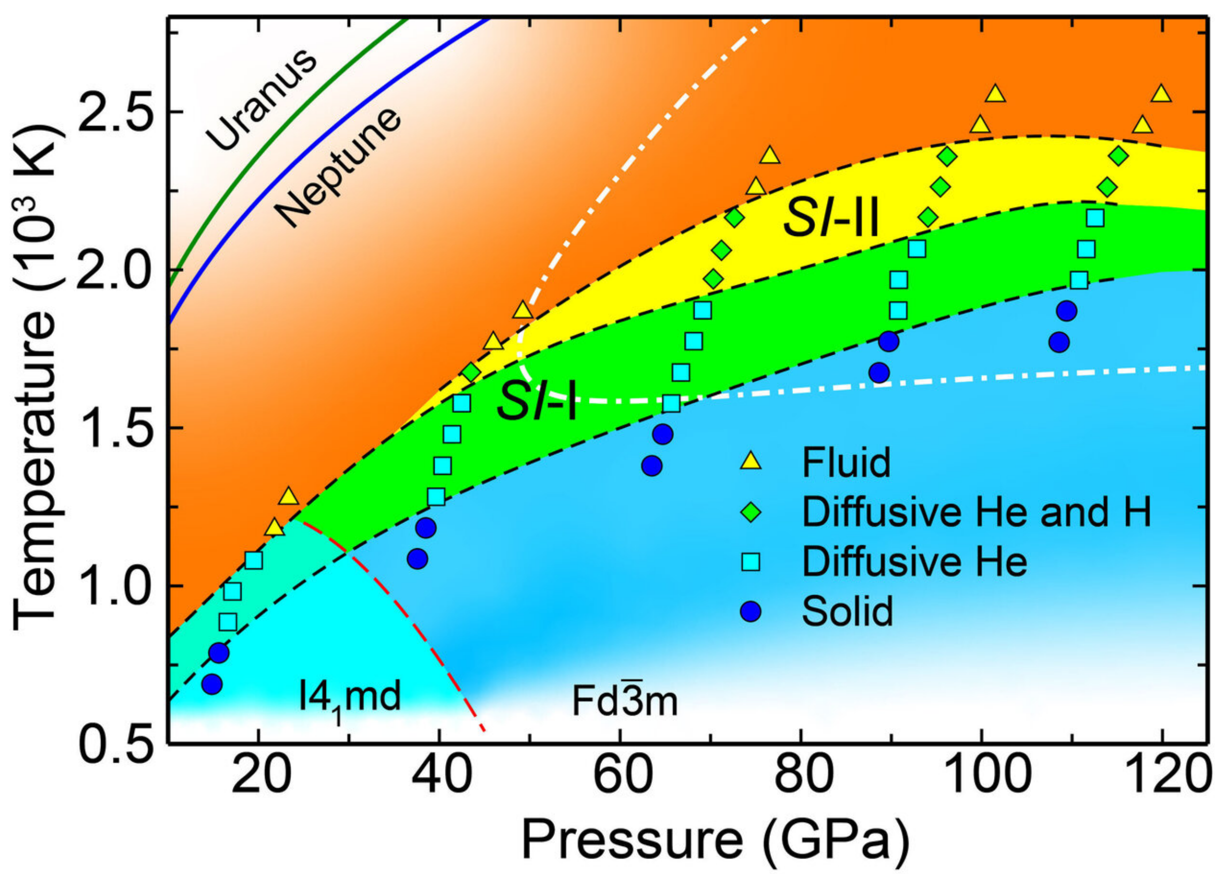
Helium and water are known to be abundant throughout the universe, particularly in giant planets such as Uranus and Neptune. Although helium is typically unreactive at common atmospheric conditions, past studies have found that it can sometimes react with other elements and compounds under high pressure.

Researchers at Nanjing University and the University of Cambridge have recently carried out a study investigating the reaction between helium and water under high pressure conditions such as those on other planets. In their study, featured in *Nature Physics*, they unveiled two previously unknown types of superionic states, which they refer to as SI-I and SI-II. Superionic states are essentially phases of matter in which a compound can simultaneously exhibit both some properties of a liquid and a solid.

"Helium is the most inert element in the periodic table and generally considered to be unreactive under ambient conditions," Jian Sun, one of the researchers who carried out the study, told Phys.org. "However, helium has been found react with some elements and compounds at high pressure. We wanted to understand whether helium and water can react with each other under high pressure and the nature of the states that may emerge under planetary conditions."

In recent years, superionic states have become a topic of interest for many research teams worldwide. A known example of these states is superionic water (or ice), a phase of water that occurs at very high temperatures and pressures at which hydrogen atoms can move freely and oxygen atoms are fixed in their sublattice.

In their study, Sun and his colleagues used calculations to show that helium (He) and water (H_2O) can form several stable compounds, which exist in a wide range of pressure conditions (from 2–92 GPa). Interestingly, they found that at high pressures and temperatures, these compounds can form superionic states that have never been observed before.



Proposed phase diagram of the helium–water system at high pressures obtained from the researchers’ structure searches and AIMD simulations. The symbols represent four distinct thermodynamic states sampled in their simulations: circle, solid state; square, He diffusive state (SI-I); diamond,both He and H diffusive state (SI-II); and triangle, fluid state. The black dashed lines were fitted to the phase boundaries. The red dashed line distinguishes the two predicted solid phases: I41md and Fd3m, as well as two types of H2O sublattice (I41md and Fd3m) in the SI-I region. Credit: Liu et al.

"We first used crystal structure search methods based on quantum mechanics to discover the most stable helium-water compounds under high pressure," Chris Pickard, another researcher involved in the study, told Phys.org. "We then performed extensive ab initio molecular dynamics simulations at high pressure and temperature to explore the states of these compounds at planetary conditions."

As a final step in their study, the researchers analyzed the superionic properties of helium-water compounds based on the simulations they performed. This ultimately allowed them to produce a pressure-temperature phase diagram for each of these compounds. Their analyses of helium-water compounds at different pressure and temperature conditions unveiled the two previously unknown types of superionic states.

"In the first of these states, the helium atoms exhibit liquid behavior within a fixed ice-lattice framework, which we named it SI-I," Richard Needs, another researcher involved in the study, told Phys.org. "In the second phase, both helium and hydrogen atoms move in a liquid-like fashion within a fixed oxygen sublattice, which we named SI-II. We found that the insertion of helium substantially decreases the pressure of superionic states compared with pure water."

The findings gathered by Sun, Pickard, Needs and the rest of their team could have several practical implications. For instance, they could help to improve our current understanding of helium compounds, the melting process of matter and the internal structure of giant planets.

"We will now study other helium compounds, especially the ones that connect directly with planetary science, such as ammonia or methane," Sun said. "We are looking for unexpected results in the universe, which provides enormous possibilities."

More information: Cong Liu et al. Multiple superionic states in helium–water compounds, *Nature Physics* (2019). DOI: 10.1038/s41567-019-0568-7: www.nature.com/articles/s41567-019-0568-7