Novel forms of the elements predicted by simulation

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The Periodic Table of elements is the basis of chemistry. Yet, it is known that the behaviour of the elements – and their chemical properties – change significantly under pressure.

Normally inert platinum and xenon become highly reactive, potassium becomes a transition metal, while hydrogen, oxygen and sulphur become superconductors. High pressure is a route to prepare novel materials with exotic structures and properties, and such materials greatly extend our understanding of the chemical bonding between the atoms. However, high-pressure experiments are very difficult and often do not permit the determination of structure.

Recently, Artem R. Oganov and Colin W. Glass from the Laboratory of Crystallo¬graphy of ETH Zurich developed a novel simulation methodology based on the laws of quantum mechanics and allowing one to predict the structure of a material at any pressure-temperature conditions given just the chemical formula.

Now they apply it to a number of chemically interesting systems including a series of chemical elements under pressure. This study – presented in the *Journal of Chemical Physics* – resolves several debates that continued over the last few decades and indicate a class of potentially technologically useful carbon-based materials.

Hydrogen – complex behaviour of the simplest

element

Hydrogen is the most abundant element in the Universe. In the Periodic Table its position is ambiguous – it can be placed either with alkali metals or with non-metallic halogens. Metallization of hydrogen under pressure is invoked to explain the magnetic fields of the giant planets Jupiter and Saturn.

It is believed that metallic hydrogen should be a superconductor up to record high temperatures (perhaps 300C). However, the structure of hydrogen at very high pressure is unknown. It is commonly believed that it should transform into a molecular metal at around 3.5 Mbar, and then turn into a non-molecular metal at ~5 Mbar. Now, ETH researchers Oganov and Glass predict that the molecular state will survive at least up to 6 Mbar. For comparison: the much stronger nitrogen molecule is destroyed at much lower pressures of ~0.5 Mbar. This puts hydrogen much closer to halogens than to alkali metals.

Unique structures of red and black oxygen clarified

It is known , that dramatic changes in the physical state of oxygen occur under pressure – from light- blue magnetic material it turns deep-red and non-magnetic. Then, at even higher pressures, it transforms into a black superconducting substance. Using their new simulation method, Oganov and Glass could clarify the unique structures of the red and the black oxygen.

Oxygen retains the O_2 molecules, but weak bonds develop also between the molecules, producing exotic chains of molecules and other molecular aggregates (e.g. pairs of molecules). Increasing intermolecular interactions under pressure are the key to understanding the change of the colour and electrical conductivity.

Towards new materials

Carbon is notorious for the variety of chemical bonds it can adopt. This chemical flexibility makes carbon very suitable for its role as the element of life. Different structures of carbon e.g. graphite, diamond, or fullerenes possess remarkably different properties. Using their simulation technique, ETH researchers have predicted several new forms of carbon at atmospheric pressure.

Two of these are especially interesting in that they contain elements of both the graphite and the diamond structures and can be expected to possess unique hardness and electrical properties. Like fullerenes, these forms would require special conditions of synthesis – but once prepared, could become technologically important materials.

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