Researchers shed light on physical properties of carbon at extreme conditions

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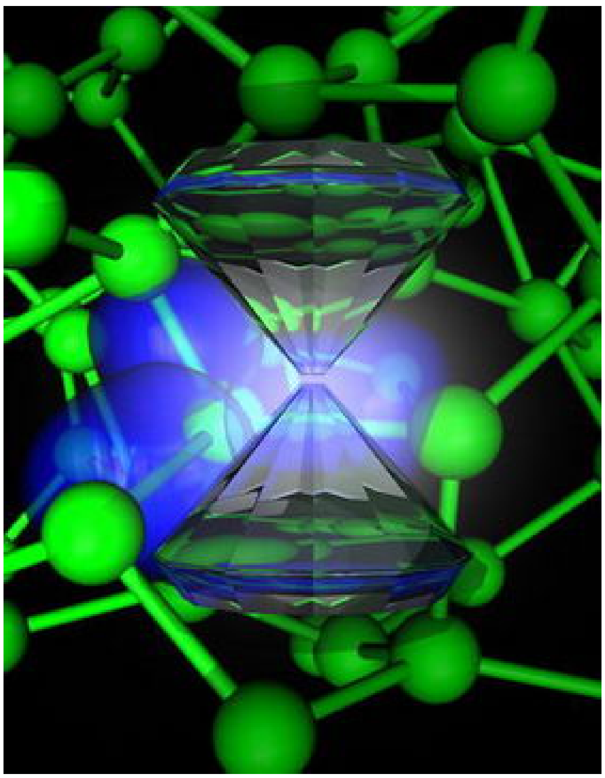

Graphic simulation of the electronic wave function (MLWF) in liquid carbon at a temperature of 9,000°Kelvin and five million atmospheres of pressure, showing a persistent covalent bonding even under these extreme conditions. At this pressure diamond melts at about 8,000°K.

A team based in Livermore has shed some light on the phase diagram of carbon at high pressure and temperature. In particular, the authors determined the solid/liquid and solid/solid phase boundaries for pressures up to 20 million atmospheres and more than 10,000 degrees Kelvin.

The simulations provide results on the physical properties of carbon, which are of great importance for devising models of Neptune, Uranus and white dwarf stars, as well as of extrasolar carbon-rich planets.

In its elemental form, carbon is found in coal, graphite, diamond, bucky balls and nanotubes. These are materials with very different properties, yet at the microscopic level they only differ by the geometrical arrangements of carbon atoms.

Elemental carbon has been known since prehistory, and one of its best known forms, diamond, is thought to have been first mined in India more than 2,000 years ago. The properties of diamond and its practical and technological applications have been extensively investigated for many centuries.

In spite of many investigations over centuries, and of important experimental work of the last decades aimed at studying compressed diamond, the phase boundaries and melting properties of elemental carbon are poorly known, and its electronic properties are not well understood under extreme conditions. Experimental data are scarce because of difficulties in reaching megabar (1 million atmospheres) pressures and thousands of Kelvin regimes in the laboratory.

The team is composed by Alfredo Correa, Stanimir Bonev and Giulia Galli who all were at the Lawrence Livermore Laboratory at the time this work started. Galli is now a professor at UC Davis and Bonev is an assistant professor at Dalhousie University, in Canada.

"Our results show a consistent description of elemental carbon in a broad range of temperature and pressures and a description of its electronic properties within the same framework," said Correa, a Student Employee Graduate Research Fellowship (SEGRF) student from UC Berkeley who works in the Laboratory's Quantum Simulations Group in the Physics and Advanced Technology Directorate. Correa is the lead author of a paper on the recent findings that appears in the online version of the Proceedings of the National Academy of Sciences for the week of Jan. 23-27.

The researchers also discovered that the diamond/BC8/liquid triple point (the temperature and pressure at which these three phases coexist in thermodynamic equilibrium) is at a lower pressure than previously thought (BC8 denotes a solid phase of carbon which diamond transforms into above 12 Mbar, at zero temperature;). The conditions at which the triple point is found are close to recent estimates of the core conditions (temperature and pressure) in Neptune and Uranus.

"Our simulation results call for a partial revision of current planetary models, especially for the description of their core regions," Correa said. "Our computational work also may help us interpret future experimental work."

Source: Lawrence Livermore National Laboratory

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