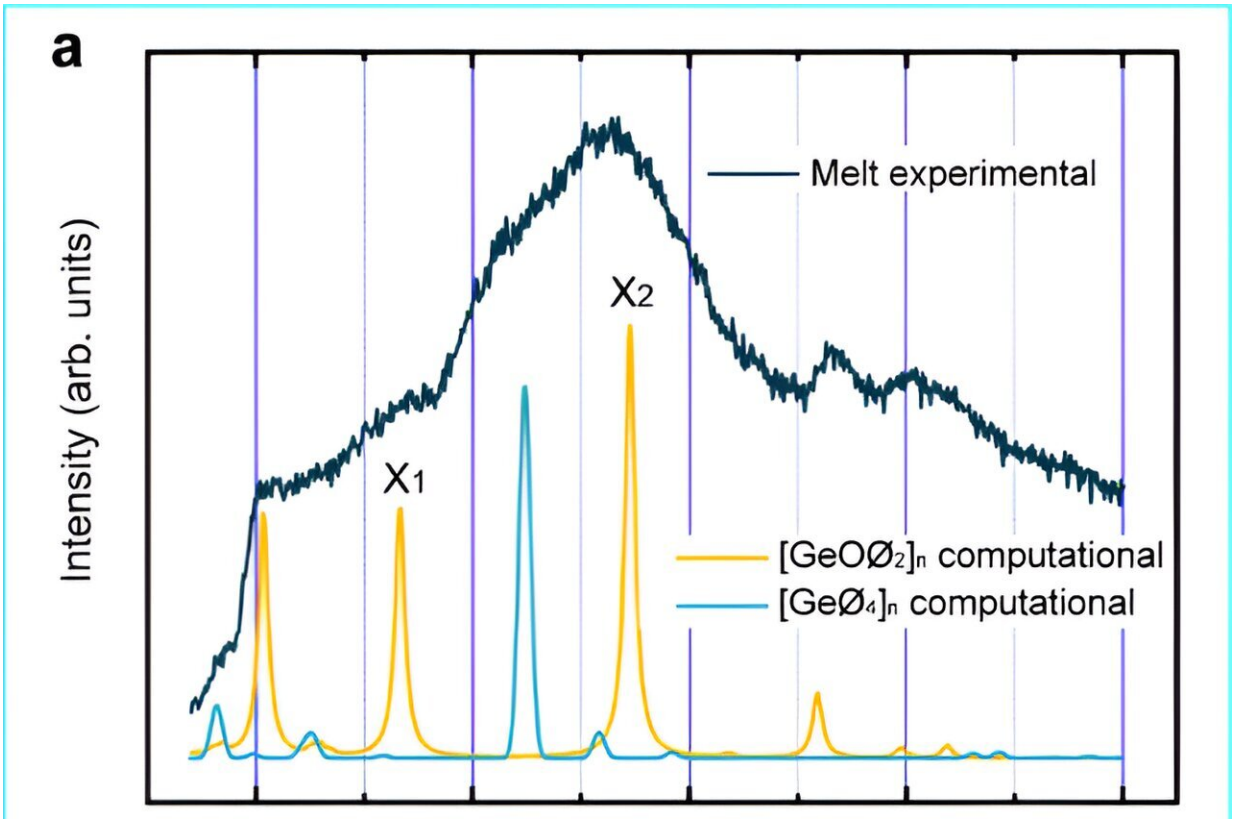
Threefold coordinated germanium proved in GeO_2 melt

December 7 2023, by Zhang Nannan



Raman spectra of the GeO_2 melt and vibrational modes of the two mysterious Raman peaks. Credit: Zheng Guimei, *Nature Communications* (2023). DOI: 10.1038/s41467-023-42890-3

According to a study published in *Nature Communications*, threefold coordinated germanium has been proved for the first time in a

germanium dioxide (GeO_2) melt, potentially resolving the long-standing debate about the structure of GeO_2 melt.

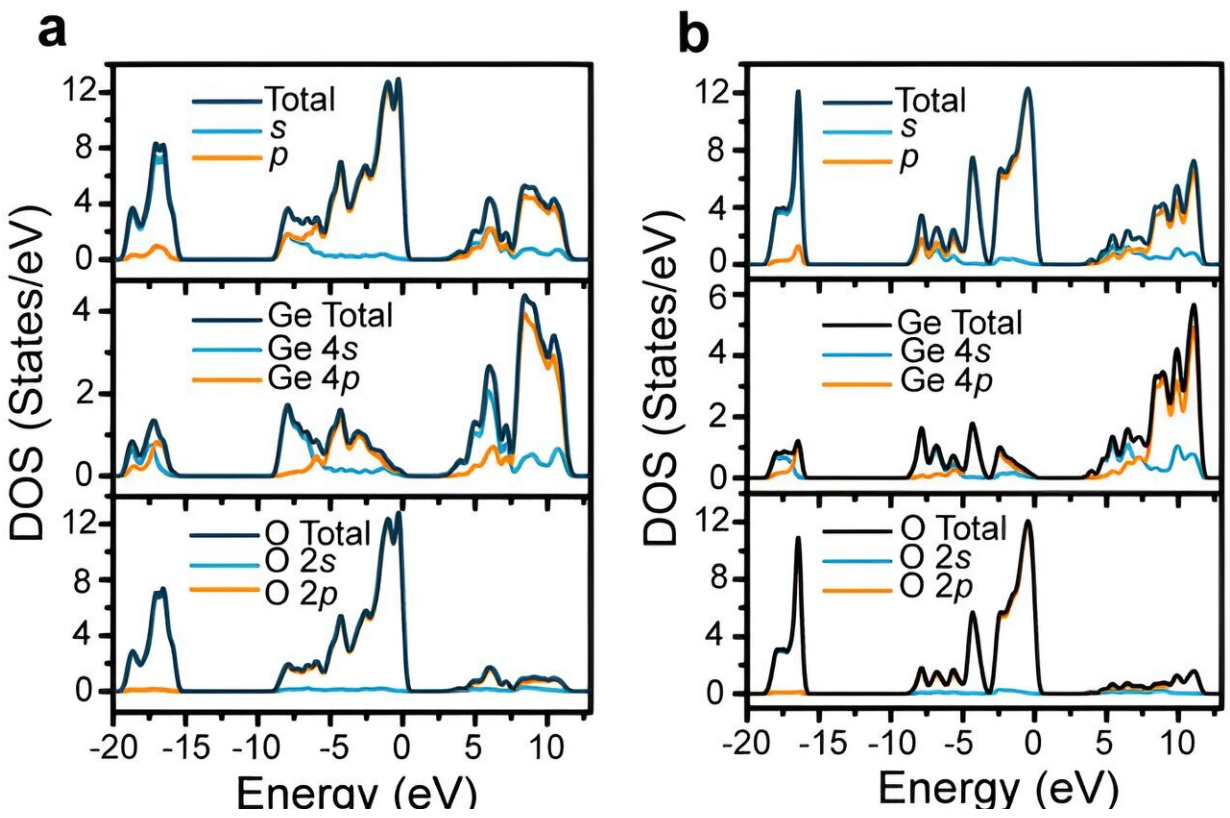
The study was conducted by a group of researchers led by Prof. Wan Songming from the Hefei Institutes of Physical Science (HFIPS) of the Chinese Academy of Sciences, in collaboration with researchers from Shanghai University.

Crystal and glass, two major states of solid, are both formed from high-temperature melts. Melt structures relate to the macro properties of melts, the micro processes of crystal growth, the formation of defects in crystals, and the structures and properties of glasses. However, the knowledge of melt structures is very limited so far due to the lack of appropriate analytical tools.

Threefold coordinated germanium is a special form of germanium bonded to oxygen, and this unique arrangement of atoms and bonds hasn't been detected in the GeO_2 melt before.

In this study, the researchers used high-temperature Raman spectroscopy and DFT calculations to investigate the structural origins of two mysterious peaks, which are located at 340 and 520 cm^{-1} in the Raman spectrum of a GeO_2 melt.

The electronic structures of the GeO_2 melt indicate that not only stable Ge–O bonds, but also fluxional Ge–O bonds exist in the GeO_2 melt, which can be used to interpret the fluidity and the viscosity of the GeO_2 melt at the molecular level.



Electronic structures of the [GeOØ$_2$]n chain and the [GeØ$_4$]n network (two building units of the GeO$_2$ melt). Credit: Zheng Guimei, adapted from *Nature Communications* (2023). DOI: 10.1038/s41467-023-42890-3

"This is how we found threefold coordinated germanium in the GeO$_2$ melt," said Wan, "and this will change the traditional view of the germanium oxide structure."

This discovery provides a new insight into the structures of germanate melts, which is helpful for better understanding the formation, defect structures, and properties of germanate crystals/glasses. In addition, as an analog of SiO$_2$, the knowledge of the GeO$_2$ melt structure also has an important implication for geological research.

More information: Songming Wan et al, Threefold coordinated germanium in a GeO2 melt, *Nature Communications* (2023). DOI: 10.1038/s41467-023-42890-3

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