Carbonia: the amorphous silicalike carbon dioxide

GORELLI F.
University of Florence, Italy

Among the group IV elements, carbon is the unique that at ambient condition forms stable double bonds with oxygen. In contrast to the cases of SiO_2 and GeO_2 the nonmolecular tetrahedral crystalline form of CO_2, phase V, only exists at high pressure. Similarly, while the amorphous phases of SiO_2 (a-silica) and GeO_2 (a-germania) are well known and stable at room condition, the amorphous, nonmolecular, phase of CO_2, although predicted by ab-initio simulations, had not yet been discovered. Here we report on the synthesis of amorphous, silica-like, carbon dioxide. The non molecular amorphous phase of carbon dioxide, a-CO_2, that for similarity with other amorphous oxide of the group IV we will call a-carbonia, was attained by compressing molecular phase III above 47 GPa at room temperature. In situ infrared spectra, measured with raising temperature up to 680 K, probe the progressive formation of C-O single bonds and the simultaneous disappearing of the molecular signatures. State-of-the-art Raman and synchrotron x-ray diffraction measurements on the temperature quenched sample show the amorphous character of this material. The comparison with vibrational and diffraction patterns of amorphous silica and germania, shows that a-carbonia is homologous to those glasses. The static structure factor of a-CO_2 has also been calculated by ab initio techniques, reproducing the main features of the experimental pattern. These findings do extend the scenario of archetypal network-forming disordered systems such as a-silica, a-germania, a-Si and a-Ge, and water.