The Study of Oxygen at High Pressure Using Inelastic X-ray Scattering

Y. Meng[1,2], H.K. Mao[2,1], P. Eng[3], J. Shu[2]

[1] HPCAT, Advanced Photon Source, Argonne National Laboratory, Argonne, IL 60439
[2] Geophysical Laboratory, Carnegie Institution of Washington, Washington D.C., 20015
[3] GSECARS, University of Chicago, Chicago, Illinois 60439

Oxygen undergoes a series of phase transitions when compressed at ambient temperature. Using inelastic x-ray scattering, we measured the K-edge spectra of O_2 from 10 GPa to 34 GPa to study the electronic bonding changes at the phase transitions. High purity oxygen was loaded into the sample chamber in an x-ray transparent beryllium gasket compressed in a diamond anvil cell (DAC). Pressure was calibrated based on ruby fluorescence scale[1]. IXS spectra were collected at station 13-ID-C of the GeoSoilEnviro Consortium for Advanced Radiation Sources (GSECARS) at the Advanced Photon Source. With a focused undulator beam to 50×15 μm at the sample, IXS measurements were performed by scanning the incident beam energy from 525 to 565 eV above the analyzer elastic scattering energy of 9.6865 keV. Scattered x-rays at the elastic energy were collected with a six-element Si (660) analyzer, positioned on the spectrometer 2-theta arm at a scattering angle of 18º, and reflected by the analyzer crystals in a near back-scattering (Bragg angle of 89°) geometry to a focused spot on an AMPTEK Si detector. The combined energy resolution of the experimental instrument is approximately 1 eV. An improved signal to background ratio was achieved by using a post-sample slit at the 2-theta angle to discriminate the single along the beam direction. Our results reveal a pressure-induced electron charge transfer into the half-filled $1\pi_g$ orbital of O_2 molecules. The high-pressure ε phase displays strong intermolecular interactions; however, the half-filled$1\pi_g$ orbital is not filled at pressures well within the stability region of the ε phase.