# Oxygen environment in lithium borates and silicates: an experimental and theoretical study.

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**Abstract**

In crystalline, glassy and liquid oxides, either bridging (BO) or non-bridging (NBO) sites are observed depending on their connectivity to the network. NBOs are defined as oxygen atoms bound to only one framework cation (Si, B, P, ...) and bearing a negative charge. The NBO concentration is an indicator of the network connectivity which influences the physical and chemical properties.
X-Ray Raman Spectroscopy (XRS) has been recently used to carry out investigations on oxygen environment under extreme conditions (pressure / temperature) [1],[2],[3] Recently, a spectral signature of NBOs at the O K-edge spectrum in lithium borates (Fig. 1) has been evidenced and validated by DFT calculations. Such signature can be used as a probe of the polymerization degree of the glass during *in situ* high-pressure / high-temperature experiments. Thanks to the recent implementation of XRS in the module XSpectra of Quantum Espresso, we are now able to understand the fine structures of the edge in terms of oxygen environment in alkali borates and silicates.

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