



# Frontiers of high pressure X-ray absorption spectroscopy

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EDITORIAL

## Frontiers of high pressure X-ray absorption spectroscopy

X-ray absorption spectroscopy (XAS) has been applied in high pressure research for decades. The unique properties of XAS, namely, chemical selectivity and sensitivity to local, electronic and magnetic structure, not only make this method very complementary to the more commonly used diffraction techniques, but also provide information on compressed matter that cannot be obtained by other methods. However, it has not seen the same level of activity or exposure of diffraction techniques. Experimentally, strong anvil absorption at low resonant energies and Bragg peak contamination from single crystalline anvils have been important limiting factors. Limited brilliance of synchrotron radiation sources have imposed constraints on the time scale over which dynamical response could be measured. Intrinsic limitations in energy resolution due to core-hole lifetime broadening have obscured the amount of detail with which electronic structure can be resolved. Interpretation of XAS data has relied on the accuracy of state of the art theoretical calculations, an additional challenge.


Emerging technologies have made possible technical advances that are rapidly changing this landscape. Diamond anvil drilling/cutting technologies now allow creating tailored anvil designs for low energy or other targeted applications. Diamond Anvil Cell (DAC)/anvil designs with large angular acceptance now enable simultaneous XAS and XRD measurements at resonant energies. Advances in synthesis of nano-polycrystalline diamond anvils allow avoiding contamination from anvil Bragg peaks, critical for extended X-ray absorption fine structure (XAFS) measurements. Advances in crystal analyzers now allow detection of X-ray emission or inelastically scattered photons with high energy resolution allowing studies of electronic structure and excitations with unprecedented resolution. For example, large area analyzer crystals combined with brilliant hard X-ray sources make it possible today to measure the carbon or the oxygen K-edge at high pressure by means of hard X-ray 'energy-loss spectroscopy' (a.k.a. X-ray Raman), thereby breaking the absorption barrier of the high pressure cell at these low energy edges. Detector technology has evolved to a point that a single 100 ps X-ray bunch can be efficiently captured amongst the train of bunches in the storage ring and used to probe ns-lived states of dynamically compressed matter. Advances in theoretical calculations now provide a more robust framework for interpretation of core-hole spectroscopies. New opportunities for static/dynamic high-pressure research are on the horizon with the advent of higher brilliance storage ring sources and expansion of X-ray free electron laser sources.

We invite you to explore in this Special Issue of 'Frontiers of High Pressure XAS' how these technical developments have enabled new scientific breakthroughs. We have tried to collect work across different continents and scientific areas. We have organized the issue as follows. Section one illustrates technical advances in anvil design for low energy XAS (Wilhelm), targeted applications (Anderson), and Bragg-peak-free XAS (Ishimatsu, Rosa). Section two captures the rapid advances in XAS-based techniques X-ray emission spectroscopy (XES) (Xiao, Yamaoka), resonant inelastic X-ray scattering (RIXS) (Rueff, Kim), and X-ray Raman (Hiraoka, Sternemann) as applied to high pressure science. Section 3 includes time-resolved XAS for studies of dynamically compressed matter at large laser facilities (Ping) and synchrotrons (Mathon, Dewaele, and Niwa). The last section highlights the unique properties of X-ray

absorption for high-pressure studies of local electronic and structural order, especially when multi-modal measurements are pursued. Articles in this section describe the combined use of XAS and XRD to probe response at multiple length scales (Itie, Fabbris), X-ray absorption near edge structure (XANES)/X-ray magnetic circular dichroism (XMCD) measurements at low temperatures as a probe of electronic structure and magnetism (Baudelet, Souza-Neto, Matsubayashi) and high temperature (> 3000 K) XAFS measurements for *in situ* investigations of the local structure of molten metals and minerals at conditions of Earth's interior (Torchio).

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