Studying soft X-ray absorption edges under extreme conditions

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The study of absorption edges has proven a powerful tool to investigate the local and electronic structure of materials. [1] Absorption edges of medium or high Z elements can be accessed using X-ray absorption spectroscopy even under extreme conditions. However, the *in situ* study of low Z elements absorption edges under extreme conditions, i.e. high temperature and high pressure, is not feasible using soft X-rays or electrons as probe. Here, non-resonant X-ray Raman scattering (XRS) as an energy loss technique enables one to choose the energy of the primary X-ray beam freely and thus gives access to shallow absorption edges even in highly absorbing sample environments such as diamond anvil cells. [2]

In this contribution we enlighten the approach of XRS as a tool to access shallow absorption edges under extreme conditions and present first results of *in situ* studies of solids and liquids under high temperature and high-pressure conditions. In particular, the Ba N_{45} - and Si L_{23} -edges of the silicon clathrate Ba_8Si_{46} was studied at pressures up to 19.4 GPa. Data of the Si and Al L_{23} -edges of hydrous sodium silicate and alumosilicate glasses are presented and compared to the first *in situ* high pressure - high temperature data on hydrous silicate melts. In addition, the O K-edge of supercritical water was studied to acquire insights into its local structure. Finally, the potential of XRS for determining the Fe oxidation state from the Fe L and/or M-edge is explored.

[1] D.C. Koningsberger, & R. Prins (1988) X-Ray Absorption, Principles, Applications, Techniques of Exafs, Sexafs & Xanes, Wiley & Sons. [2] W. Schülke (2007) Electron Dynamics by Inelastic X-Ray Scattering, Oxford University Press.

An oxygen window for early Ediacaran animal life

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Complex multicellular organisms including early metazoans appeared in the Ediacaran Period shortly after the termination of the late Cryogenian (Marinoan) glaciation about 635 million years (Myr) ago. Given that metazoans have high respiratory demands, it has been speculated that the termination of the Marinoan glaciation, the rise of oxygen, and evolution of complex life forms were casually linked. Previously published geochemical data, however, suggest that a major increase in the extent of ocean oxygenation did not happen until the middle Ediacaran Period, 50 Myr after the first appearance of animal fossils. This later oxygenation is arguably linked to the termination of a much less severe Gaskiers glaciation around 580 Myr ago. Here we report new geochemical data from early Ediacaran (ca. 632 Myr ago) organic-rich black shales of the basal Doushantuo Formation in South China. Iron speciation and sulfur isotope data indicate pervasive deep-water euxinia (anoxic and sulphidic) and an increase in the marine sulphate reservoir from the oxidative weathering of crustal sulphides. High molybdenum (Mo) and vanadium (V) enrichments (Mo: 120 parts per million [ppm] and V: 6000 ppm) in these shales record an increase in the oceanic Mo and V reservoirs and hence point toward a significant post-glacial oxygenation event. Our data provide evidence for co-evolution of marine redox conditions and early animals in the immediate aftermath of the Marinoan glaciation.

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