BioXAS to watch biological catalysis

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Understanding structure-function relations is one of the main interests in the molecular biosciences. X-ray absorption spectroscopy on biological samples (BioXAS) has gained the status of an useful tool for characterization of the structure of protein-bound metal centers. The method is well-suited for investigations on the particularly interesting changes in electronic structure (oxidation states) and atomic structure (arrangement of ligand atoms) of the metal center which typically accompany transitions between various 'states' of the metal site. Due to the progress in the performance characteristics of synchrotron radiation sources and of experimental stations dedicated to the study of (ultra-dilute) biological samples, it is now possible to carry out new types of BioXAS experiments which have been impracticable in the past. Of particular interest are approaches to follow biological catalysis at metal sites by characterization of functionally relevant structural changes. First steps towards the use of BioXAS to 'watch' biological catalysis are reviewed for the water-splitting reactions occurring at the manganese complex of photosynthesis. The following aspects are considered: (1.1) the Role of BioXAS in life sciences; (1.2) BioXAS - methodical aspects; (1.3) catalysis at the Mn complex of photosynthesis; (2.1) combination of EXAFS and crystallographic information; (2.2) freeze-quench technique to capture semi-stable states; (2.3) time-resolved BioXAS using a freeze-quench approach; (2.4) room-temperature experiments and 'real-time' BioXAS; (3) tasks and perspectives.