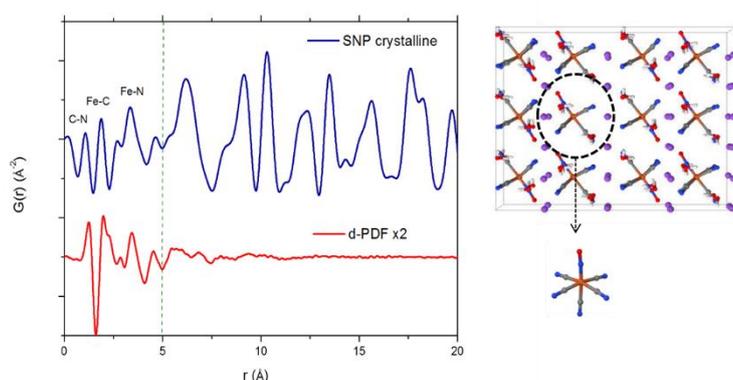


## Impact of the confinement on physiological liquids in bioactive glasses: structure – property relationship

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Significant therapeutical progress has been achieved in recent years by using bioactive glasses for bone repair and replacement. These materials are more and more studied in view of their frequent application in orthopedic and reconstructive surgery. The interest in bioactive glasses stems from the fact that in contact with biological matter they develop rapidly surface layers of hydroxyapatite which allows to adhere to the biological substrate and hence to reconstruct damaged bones. The internal porosity of these biomaterials further allows for progressive colonization of the tissues, ensures the vascularization and free circulation of cells, body fluids and nutriment. The understanding of the impact of the confinement on the organization and diffusion of the physiological liquids encapsulated in these bionanomaterials is thus crucial for improving the bioglasses' properties. The detailed structural analysis of this kind of nanomaterial can be performed by total X-ray scattering and solid-state nuclear magnetic resonance (NMR). In this context we develop since several years a combined X-ray – NMR methodology allowing for a thorough structural characterization of porous nanomaterials and the embedded guest molecules [1,2]. The method is based on the multiscale modelling (from sub-Angstrom to several tens of nanometers) of total X-ray scattering data using the pair distribution function (PDF). The PDF analysis allows for the determination of the structural parameters on a local and intermediate scale and hence the study of ordering effects due to confinement. Complementary information is obtained from solid-state NMR, namely concerning the local structure and light elements such as hydrogen. Further NMR enables also the study of dynamical behavior of the encapsulated species.

The thesis project contains a significant experimental part, consisting in collecting and analyzing total X-ray scattering data from laboratory and/or synchrotron experiments as well as neutron diffraction experiments. Further complementary experimental techniques employed are solid-state NMR, NMR relaxometry, and differential scanning calorimetry. An important part of the project is based on Monte Carlo simulation for the reconstruction of the different structural models.



**Figure:** Pair distribution function  $G(r)$  obtained for an iron complex in bulk form and from the isolated species embedded in a porous host [2]

**References:**

- [1] E.-E. Bendeif et al., RSC Advances 5, 8895 (2015)
- [2] K.-Y. Hsieh et al., RSC Advances 3, 26137 (2013)

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