STRUCTURAL STUDY OF THE LOCAL ORDER IN AMMONIA-MODULATED FE(II) HYDROXYPHOSPHONOACETATE PROTON CONDUCTORS

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Layered Fe(II) carboxiphosphonate, Fe-HPAA·$2H_2O$[1], is a crystalline multifunctional coordination polymer exhibiting properties as photocatalyst[2] and proton conductor. Post-synthesis modification by ammonia/water adsorption[3] strongly enhances its proton conductivity. However, this process entails a progressive amorphization but in no case intercalation of the guest species was detected. Understanding the mechanism involved in this increased conductivity is crucial to develop novel high performance proton conductors for PEMFCs. Thus, total scattering and PDF study has been carried out to explore the mechanism of ammonia adsorption and subsequent amorphization.

Different lenght scales have been investigated to characterize the average and local structure at variable ammonia loaded in order to ascertain posible structural modifications after gas/solid reactions. While significant short range order (from 1.4 to 10 Å) variations were observed even for low loadings, the average structure seems to be basically preserved except for the highest ammonia/water contents.

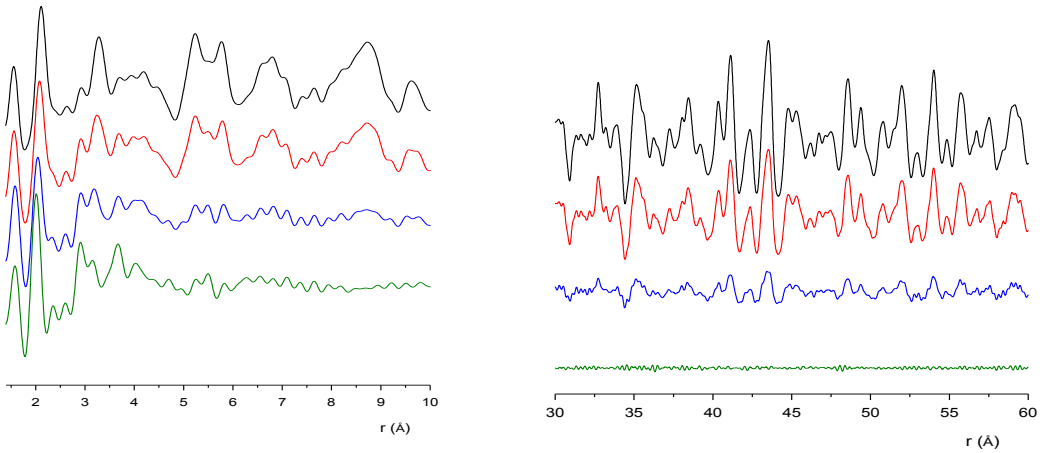

Figure 1. Radial distribution functions for FeHPAA exposed to NH_3 gas at several times (0h black, 36h red, 48h blue and 72h green)

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[1] R. Fu, S. Xiang, H. Zhang, J. Zhang, and X. Wu, *Cryst. Growth Des.***2005**, *5,* 1795-1799.
[2] M Bazaga-García, A. Cabeza, P. Olivera-Pastor, I. Santacruz, R. M. P. Colodrero, and M. A. G. Aranda, *J. Phys. Chem. C* **2012**, *116*, 14526−14533.
[3] M. Bazaga-García, R. M. P. Colodrero, M. Papadaki, P. Garczarek, J. Zoń, P Olivera-Pastor, E. R. Losilla, L. Le n-Reina, M. A. G. Aranda, D. Choquesillo-Lazarte, K. D. Demadis and A. Cabeza *„J. Am. Chem. Soc.* **2014**, *136*, 5731−5739.