

## Determination of Surface Reactivity of Inorganic Anion Exchangers Based on Complex Metal Hydrous Oxides Using EXAFS Simulation

N. Chubar<sup>1</sup>, V. Gerda<sup>1</sup>, G. Yablokova<sup>2</sup>, D. Banerjee<sup>3</sup>

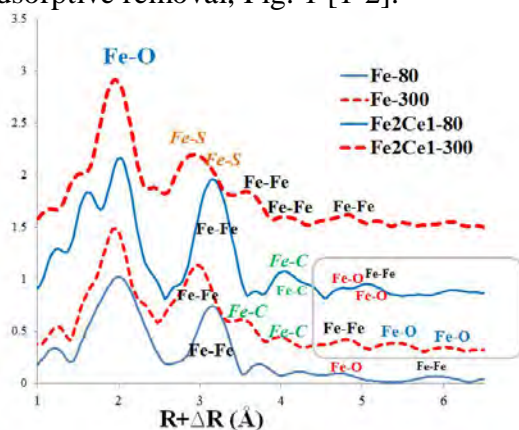
<sup>1</sup>Taras Shevchenko National University of Kyiv, Faculty of Chemistry, 01601, Ukraine

<sup>2</sup>KU Leuven, Department of Materials Engineering, 3001 Leuven, Belgium

<sup>3</sup>Dutch-Belgian Beamline (DUBBLE), ESRF – The European Synchrotron CS 40220, Grenoble, France

Many emergent functions have been discovered at the interfaces of complex metal oxides, including such promising compositions as hydrous oxides of d-metal + lanthanide, Fe-Ce, and their composites. Success in applications of these materials in adsorption and catalysis depends on their structural and electronic properties which can be fully investigated by synchrotron-based techniques, such as EXAFS (X-ray absorption fine structure)/XANES (X-ray absorption near edge structure) that covers both crystalline and amorphous phases and provide new insight into the structure of complex oxide-based materials.

To gain deeper insight on adsorptive reactivity of Fe-Ce oxide-based composites (hydrothermally precipitated at Fe-to-Ce dosage ratios of 1:0, 2:1, 1:1, 1:2, and 0:1) their atomic-scale properties at synthesis [1] as well as their reconstruction processes upon treatment at 300°C [2] were investigated by EXAFS/XANES, XRD, XPS and FTIR. The structural changes were correlated with the adsorptive removal of arsenate, phosphate, fluoride, bromide, and bromate which are the target anions for water treatment industries. In spite of general awareness of the importance of surface area in adsorptive removal, the increase in surface area upon thermal treatment did not increase adsorption of the studied anions. However, EXAFS simulations and the adsorption of most of the anions provided evidence of regularities between local structures around Fe atom in composites treated at 80 and 300°C. The best adsorption of most anions was demonstrated by adsorbents whose simulated outer Fe shells resulted from oscillations from both O and Fe atoms. In contrast, the loss of extended local structures at >4 Å was correlated with the decrease of adsorptive removal, Fig. 1 [1-2].



Radial structure around Fe, obtained from Fourier transforms of Fe K-edge EXAFS oscillations of the samples and fitting results.

For the first time, the utilization of EXAFS to obtain an extended local structure has been suggested as a methodological approach to estimate the surface reactivity of inorganic materials based on metal hydrous oxides intended for use as anion exchange adsorbents and possibly catalysts.

- [1] N. Chubar, V. Gerda, D. Banerjee, Influence of 300 °C thermal conversion of Fe-Ce hydrous oxides prepared by hydrothermal precipitation on the adsorptive performance of five anions: Insights from EXAFS/XANES, XRD and FTIR (companion paper), *J. Colloid Interface Science* **491**(1) (2017) 111-122.
- [2] N. Chubar, V. Gerda, D. Banerjee, G. Yablokova, Effect of Fe(II)/Ce(III) dosage ratio on the structure and anion adsorptive removal of hydrothermally precipitated composites: Insights from EXAFS/XANES, XRD and FTIR, *J. Colloid Interface Science* **487**(1) (2017) 388-400.