

**Adsorption properties of nanostructured hybrid materials based on
NHC=OO functionalization modified by boron and zirconium – a
comparative study**

Ralitsa Georgieva¹, Paunka Vassileva¹, Albena Detcheva¹, Dimitrinka Voykova¹, Tsvetelina Gerganova² and Yordanka Ivanova²

¹Institute of General and Inorganic Chemistry, Bulgarian Academy of Sciences, 1113 Sofia, Bulgaria. *E-mail:* albena@svr.igic.bas.bg

²University of Chemical Technology and Metallurgy, Department of Silicates, 1756 Sofia, Bulgaria

The adsorption properties of two new nanostructured hybrid materials containing B₂O₃ and ZrO₂ were studied and compared. The new organic-inorganic nanostructured materials were synthesized via a sol-gel method through hydrolysis and co-condensation reactions using trimethylsilyl isocyanate as a new silica source in the presence of tetramethoxysilane. As a modifying agent a quantity of 10 wt.% Zr(OPr)₄ or B(OCH₃)₃ was added. The structure of the hybrid materials was investigated by means of XRD and FTIR. Based on the data of the analyses pointed out the most probable cross-linking mechanism for the derived gels was proposed. The characterization of porous and texture parameters of both materials was carried out by low-temperature adsorption of nitrogen. The nitrogen adsorption isotherms were analyzed to evaluate the following parameters: the specific surface area, the total pore volume and average pore diameter.

Adsorption of Cu(II), Fe(III), Cr(III), Cd(II) and Pb(II) ions on both materials was investigated using multi-component solutions with different concentrations and acidity by means of the batch method. The adsorption was significantly affected by the pH value. Equilibrium modeling data were fitted to linear Langmuir, Freundlich and Dubinin-Radushkevich models and maximum adsorption capacities were calculated. In the present study, best fitting was observed by the Langmuir model, which showed correlation coefficients of greater than 0.95 for both systems studied. Thus we proved that Langmuir isotherm most adequately described the adsorption processes of the investigated ions. Kinetic of multi-component solutions at 0.5h, 1h, 5h and 24h was investigated. Pseudo-first order, pseudo-second order and intraparticle diffusion models were used to analyze kinetic data. The static capacities for multi-component solutions of the investigated ions were calculated. Both materials showed good adsorption properties towards Cu(II), Fe(III), Cr(III), Cd(II) and Pb(II) ions but the boron-containing material proved to be more suitable for their removal from aqueous solutions.