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ABSTRACT BOOK

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Study of Zr-based metal-organic frameworks for water remediation

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MOFs are a class of crystalline inorganic-organic hybrid porous materials which show large surface areas, high porosity and easy chemical tunability. The MOFs are produced by a coordination reaction between metal clusters and organic ligands.[1] The interest on these compounds is mainly due to the outstanding physical properties they show, which allow them to access many different uses of applications (gas separation, catalysis, biomedical imaging etc).[2] MOF-801 and MOF-808 are two Zr-based MOFs which have shown a high chemical stability. Therefore, we have studied the adsorption capacity of both compounds towards the adsorption of Cr(VI) from water.

Kinetic experiments for MOF808 showed that the maximum amount of Cr(VI) ions was adsorbed within the first 15 minutes (63% of total metal ions adsorbed at 50ppm and 30% at 100ppm), while for MOF801 a 20% of the metal anions are captured during the first 30 minutes of the kinetic experiment.

In order to understand the Cr(VI) adsorption capacity and affinity by the MOF materials, we have construct the adsorption isotherms for both compounds, analyzing the data with Langmuir and Freundlich adsorption isotherm models, concluding that MOF-801 has a better affinity towards the adsorbate than MOF-808.

The influence of the pH of the solution has been also studied its effect not only on surface charge of the adsorbent, but also on the degree of ionization and speciation of adsorbate.[3] The better results were observed for MOF-808 at pH 3.5.

The materials have been characterized after the adsorption processes, to confirm that the structural and chemical properties of the MOFs are equal to the fresh material, by means of X-ray diffraction, IR spectroscopy and X-ray photoelectron spectroscopy.

Finally, an adsorption mechanism for Cr(VI) onto the Zr 12-c ideal clusters has been proposed.

References

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