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Short communication

Experimental and molecular modelling approach for rapid adsorption of Bisphenol A using Zr and Fe based metal–organic frameworks

Afzan Mahmad [a,b], Maizatul Shima Shaharun [a], Teh Ubaidah Nak [c], Zakariyya Uba Zango [a,d], Mohd Faisal Taha [a]

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Abstract

The synthesized highly porous functionalized metal–organic frameworks (MOFs) are the solution for the rapid removal of toxic pollutants from wastewater. Bisphenol A (BPA) which consists of a derivative of phenol was identified as the primary pollutant in environmental waters and requires elimination for a sustainable and greener environment. In this work, we reported highly porous and stable Zr and Fe–based metal–organic frameworks as adsorbents for the removal of BPA in an aqueous solution. In this study, MIL–88(Fe) (MIL stands for Matériaux de l'Institut Lavoisier) and UiO–66(Zr) (UiO stands for University of Oslo) were synthesized by solvothermal techniques and characterized by fourier transformed infrared spectroscopy (FTIR), x–ray diffraction (XRD), energy–dispersive x–ray spectroscopy (EDX), field emission scanning electron microscopy (FESEM), scanning electron microscopy (SEM) and nitrogen adsorption–desorption measurements. MIL–88(Fe) and UiO–66(Zr)had 1242 and 1421 ng^2/g surface area, respectively. In the experimental study, the UiO–66(Zr) and MIL–88(Fe)removed 99.25 and 98.36 % BPA, respectively. Compared to MIL–88(Fe), UiO–66(Zr) showed faster adsorption of BPA. The process was exothermic and spontaneous. The pseudo–second order model suited the kinetics studies well, while the Langmuir model fit the MIL–88(Fe) and UiO–66(Zr)isotherms. Molecular docking was used to study the surface interactions of MIL–88(Fe) and UiO–66(Zr) with BPA.The process involved van der Waals and hydrogen interactions between BPA with MIL–88(Fe) and UiO–66(Zr) surfaces. Both MOFs proved to have high efficacy and appropriateness for the practical application of BPA adsorption from an aqueous solution.