

# **Metal–Organic Framework-74 for Ultratrace Arsenic Removal from Water: Experimental and Density Functional Theory Studies**

Belal J. Abu Tarboush, Ali Chouman, Antranik Jonderian, Mohammad Ahmad, Mohamad Hmadeh, and Mazen Al-Ghoul

Department of Chemical and Petroleum Engineering and Department of Chemistry, American University of Beirut

This study investigates and compares arsenic, As(V), removal from aqueous media using the water-stable zinc metal–organic frameworks (Zn-MOF-74) prepared via room-temperature precipitation (RT-Zn-MOF-74) and a solvothermal procedure (HT-Zn-MOF-74). The Zn-MOF-74 crystals possess average particle sizes of 66 nm and 144  $\mu\text{m}$  for RT-Zn-MOF-74 and HT-Zn-MOF-74, respectively. Moreover, nanosized RT-Zn-MOF-74 exhibited a superior performance to HT-Zn-MOF-74. While the Brunauer–Emmett–Teller surface area of RT-Zn-MOF-74 was smaller than that of HT-Zn-MOF-74, higher adsorption uptake took place on the room-temperature-synthesized ones because of their small particle size and better dispersion. Adsorption isotherm studies showed that the Langmuir isotherm was effective for the adsorption of As(V) onto RT-Zn-MOF-74 and HT-Zn-MOF-74 with maximum adsorption uptake ( $q_{\text{max}}$ ) values of 99.0 and 48.7  $\text{mg g}^{-1}$ , respectively. These values exceed most reported maximum adsorption capacities at neutral pH. The thermodynamics of adsorption revealed a spontaneous endothermic process that is due to the substitution of adsorbed water molecules by arsenate in the pores of the MOF crystal. This was further investigated using plane-wave density functional theory calculations. This study constitutes direct evidence for the importance of tuning the size of the MOF crystals to enhance their properties.