

Simulation guided prediction of zeolites for the sorption of selected anions from water: Machine learning predictors for enhanced loading

Abstract

The development of highly efficient adsorbents, especially those that can harvest anions like CrO_4^{2-} , AsO_4^{3-} , NO_3^- and PO_4^{3-} , is one of the principal challenges in the water treatment field. The current study utilized a screening process involving an initial selection of zeolites based on the pore-limiting diameter, followed by GCMC (Grand Canonical Monte Carlo) simulations to identify high-performing zeolites for anion removal. CLO, LTN, MWF, TSC, ITV, PAU, FAU and DFO zeolites are the best performing in terms of loading while several zeolites like ANA, DFT, BIK, SBN and JNT gave no loading at all. In addition, quantum chemical calculations revealed that after adsorption of the anions on the zeolite, there is charge transfer between the zeolite and the anion. The CLO cluster has a charge of 0.64 before adsorption. After adsorption, it attains a charge of -0.06 , suggesting that the phosphate ion acts as an electron donor while the CLO cluster, as an electron acceptor. Finally, machine learning was employed to rank the importance of the various descriptors that have influence on the removal of anions in water. Largest overall cavity diameter, mass and accessible pore volume appeared to be the three most important descriptors, thus, tuning the sphere cavity and inter channel diameter as well as engineering the accessible volume of zeolite architectures are of utmost important toward harvesting the desired anions.

Authors:

Fred Sifuna Wanyonyi, Timothy Tizhe Fidelis, Hitler Louis, Gershom Kyalo Mutua, Francis Orata, Lydia Rhyman, Ponnadurai Ramasami, Anthony M.S.Pembere