Role of pore chemistry and topology in the heavy metal sorption by zeolites: From molecular simulation to machine learning

Abstract

Zeolite frameworks can provide pores that enable selective heavy metals sorption, making these materials promising for energy-efficient heavy metals capture. In the present study, the adsorption of hazardous heavy metal ions on 242 zeolites have been investigated by employing molecular simulations and machine learning techniques, where the role of pores, topology, and chemical characteristics in the heavy metal sorption has been examined. The molecular simulation results show that only the zeolites with high diameter of pores exhibited appreciable loading of the cations. To unravel the encoded chemical information of the three parameters (total energy, pore size and average volume) on how each influence the loading capacity of the heavy metals, boruta algorithm; a wrapper based built around random forest classier was employed to rank these parameters. In light of the forgoing, total energy accounts for the highest contribution for the sorption of heavy metals. Compared to the pore size, the average volume was rejected by the random forest classier algorithm, which implies that the individual pore size on the surface of each of the best performing zeolite framework is responsible for the adsorption of heavy metals with relatively high sphere diameter instead of total volume of each zeolite.

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