

Unlocking the adsorptive effectiveness of naturally occurring heulandite zeolite for the removal of PO_4^{3-} and NO_3^- anions from wastewater

Abstract

The mitigation of high levels of phosphate (PO_4^{3-}) and nitrate (NO_3^-) ions in water bodies, particularly in agricultural wastewater, holds paramount importance in curbing eutrophication within aquatic ecosystems. Herein, using experimental and computational techniques, the study explored the potential of naturally occurring South Africa heulandite (HEU) zeolite for the removal of PO_4^{3-} and NO_3^- ions from synthetic wastewater in batch mode. The percentage removal of PO_4^{3-} and NO_3^- was 59.15% and 51.39%, respectively, whereas the corresponding maximum adsorption capacity of the adsorbent was 0.0236 and 0.0206 mg/g. The adsorption kinetics of both anions by HEU fitted well in the pseudo-first-order (PFO) kinetic model indicating a physisorption-mediated rate-determining step. It was revealed that the adsorption process was multi-mechanistic spontaneous and exothermic. Molecular simulations using Monte Carlo (MC) and density functional theory (DFT) methods also provided insights into the adsorption mechanisms.

DOI: <https://doi.org/10.1007/s10661-024-13522-0>

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