

A New Paradigm for Anionic Water Pollutant Adsorption: High Entropy LDHs

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Nuclear fission energy accounts for 10% of the total energy generated. As it does not emit greenhouse gases, it is considered a leading sustainable energy source. However, radioactive anions can be released through sewage, causing mutations and cancer in living organisms, which leads to severe disruption in marine ecosystems. Specifically, radioactive iodine is one of the seven long-lived nuclear fission products, with a half-life of 15.7 million years. A basic Layered Double Hydroxide (LDH) was previously developed to adsorb radioactive iodine. To address its limitations, the high-entropy effect was proposed as a solution to the challenges associated with using the basic LDH structure. High-entropy materials are composed of various elements, allowing the design of materials with high efficiency and stability suitable for specific applications. However, this approach results in an immense number of possible compositions to explore, and the limited experimental data reported so far restricts conventional exploration methods. In this study, machine learning was utilized to explore quaternary and quinary LDH compositions for radioactive iodine adsorption. As a result, $\text{Cu}_3(\text{CrFeAl})_1$ was identified as the LDH composition with the highest adsorption performance, increasing the previous maximum performance of 89.2% to 91.8%, all while exploring less than 1% of the total experimental space. This work demonstrates and analyzes high-entropy LDH with outstanding iodate adsorption performance and validates the efficiency and feasibility of this approach. It has the potential to be a pioneer in anionic pollutant adsorption materials, ultimately contributing to environmental preservation.

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