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Environmental impact of amino acids on the stability of hydrotalcite after bearing SeO_4^{2-} integrated with DFT simulation

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^{79}Se isotope as one of the radionuclides, which is produced by nuclear electricity in chemical forms of selenate (SeO_4^{2-}) and/or selenite (SeO_3^{2-}) with a half-life time of 3.27×10^5 years. ^{79}Se oxyanions can be immobilized by layered double hydroxides (LDHs) for disposal underground, which are commonly anionic exchangers in cementitious materials. The natural accidents such as earthquakes or related phenomena can disturb the resulting vault and accelerate radionuclides wastes to leach into the soil and water environment. Organic aicds might have some effects on their mobility. Amino acid is one of model of organic acids in pedosphere which are originally from degraded substances of dead soil animals and microorganisms.

In the present work, hydrotalcite (Mg_2Al-LDH) bearing SeO_4^{2-} were prepared by ion-exchanging method. Effects of several amino acids (glycine, aspartic acid, cysteine, phenelalanine, and tryptophan) on the stability of SeO_4^{2-} in Mg_2Al-LDH was explored under alkaline conditions. Glycine, aspartic acid, and cysteine have promoted the release of SeO_4^{2-} from Mg_2Al-LDH. DFT simulation confirmed glycine can be intercalated into Mg_2Al-LDH interlayer in different orientations. And Cys suppressed Mg released by forming Mg-Cys complexes.Therefore, under the alkaline geochemical environment, amino acids which have smaller molecular sizes and higher charge densities might cause the risk to release ^{79}Se from cement disposal sites and the second radionuclides contamination.