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# Atomistic computer simulation of the structure and properties of iodine and chlorine containing hydrocalumite (AFm phase) as adsorbent for radionuclides $^{36}\text{Cl}$ , $^{129}\text{I}$ , $^{137}\text{Cs}$

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AFm phases of hydrous Ca-aluminates  $\text{Ca}_2\text{Al}(\text{OH})_6\cdot\text{Cl}\cdot 2\text{H}_2\text{O}$  (also known as hydrocalumite) and  $\text{Ca}_2\text{Al}(\text{OH})_6\cdot\text{I}\cdot 2\text{H}_2\text{O}$  were considered as adsorbent for radioactive anions. The layered structure of hydrocalumite is formed by distorted Ca-hydroxide and Al-hydroxide octahedra. Its interlayers are formed by a highly ordered arrangement of Cl<sup>-</sup> anions and H<sub>2</sub>O molecules. It is structurally one of the best understood of the layered double hydroxides (LDHs) and can serve as a good model for other less ordered natural and synthetic LDH phases important for a wide variety of technological applications, such as environmental remediation, while only experimental studies of iodine-containing AFm phases have been conducted.

In this work we studied hydrocalumite with chlorine and iodine anions in interlayer space as adsorbent for radionuclides  $^{36}\text{Cl}$ ,  $^{129}\text{I}$ ,  $^{137}\text{Cs}$  via molecular dynamics simulations. Performed computer simulations allowed us to study both crystals properties and interaction of the same crystals with aqueous solutions of CsCl and CsI.

The structural and dynamic properties for both systems were modelled with the ClayFF-MOH force field model that is capable of realistically describe all interatomic interactions in such systems and which can now more accurately account for the bending of Al–O–H and Ca–O–H angles in the mineral structure. Our results are confirmed with earlier atomistic simulations of hydrocalumite which were among the first successful applications of the ClayFF force field model.

Study reported that stronger adsorption of Cl<sup>-</sup>, compared to adsorption of I<sup>-</sup>, leads to partial adsorption of Cs<sup>+</sup> cation. This can be explained by the difference in van der Waals radius of Cl and I that make up 175 pm for Cl and 198 pm for I. In addition, the diffusion decreases by an order of magnitude at a distance of 3 Å, which is consistent with previous works.

## Participation

In-Person

## References

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