

# Density functional studies for cesium adsorption to micaceous clay minerals: Low and high density situations

M. OKUMURA<sup>1\*</sup>, H. NAKAMURA<sup>1</sup> AND M. MACHIDA<sup>1</sup>

<sup>1</sup>Japan Atomic Energy Agency, Kashiwa 277-0871, Japan  
(\*correspondance: okumura.masahiko@jaea.go.jp)

Radioactive nuclides were provided into an environment by the Fukushima Nuclear Power Plant accident. Among them, radiocesium is mainly retained by surface soil. In the surface soil, micaceous clay minerals adsorb radiocesium strongly. Particularly, it is known that the edge parts of them show selective adsorption of cesium. Furthermore, a special sorption site called “frayed edge site” (FES) is considered as the origin of the selective adsorption. FES is a site located between closed interlayer with potassium and opened one with hydrated calcium or magnesium ions created by weathering. But there were no experimental and theoretical evidences that FES adsorbs cesium selectively. In order to reveal the mechanism of the selective adsorption, we made a simple FES model using density functional theory [1]. We showed that the interlayer distance of FES is critical for the selective adsorption: the cesium ion is adsorbed when the interlayer distance is enough large but is not when it is small. This is the first evidence that FES actually adsorbs cesium ions. We revealed the mechanism of this cesium adsorption by FES: a match between the interlayer distance and the ion radius.

It was expected that the density of the provided cesium in Fukushima is very low. But recent observation reported that cesium ions are accumulated by specific clay minerals, and the density is much higher than expected. In this situation, serial adsorption can reasonably occur. Then we evaluated Gibb’s free energy of serial ion exchange reaction between cesium and potassium preoccupied in micaceous clay minerals. We showed that the serial adsorption increases the affinity of clay minerals for further cesium adsorption. This result consistent with recent experimental results about high density cesium adsorption by phlogopite.

These results give fundamental information about microscopic adsorption reaction of cesium adsorption by micaceous clay minerals.

[1] M. Okumura, H. Nakamura, and M. Machida, (2013). *J. Phys. Soc. Jpn* **82**, 033802

[2] M. Okumura, H. Nakamura, and M. Machida, (2014). *Clay Science* **18**, 53-61