Numerical studies of effects of microscopic structure on affinity of clay minerals to cesium ion

M. OKUMURA[1*], H. NAKAMURA[1], AND M. MACHIDA[1]

[1]Center for Computational Science and e-Systems, Japan Atomic Energy Agency, 178-4-4 Wakashiba, Kashiwa, Chiba 277-0871, Japan (*correspondance: okumura.masahiko@jaea.go.jp)

Radioactive cesium provided by the Fukushima nuclear power plant accident is a main gamma-ray emitter adsorbed by surface soil. Many residents were evacuated from contaminated areas in Fukushima. To reduce additional radiation dose of residents when they return to their home, large-scale decontamination has been performed. As a result, huge amount of waste soil has been produced. Construction and maintenance of storage sites of the waste soil are social burdens in Japan. Then, volume reduction of the waste soil is a promising way to reduce the burden. However there is no standard efficient and economic technique. One of the reasons of it is lack of scientific knowledge about adsorption and desorption of cesium by the surface soil.

It is known that micaceous clay minerals in surface soil are main adsorbants of radioactive cesium. Recent experiment revealed that weathered biotite have strongest affinity to radiocesium among several clay minerals [1]. But mechanisms of the affinity is still unknown.

In order to reveal a mechanism of the affinity, we consider energetics of adsorption of cesium to several clay minerals using *ab initio* numerical simulation method. We show that phlogopite, an end member of biotite, is more energetically favorable than muscovite for cesium adsorption. This implies that difference of microscopic structures of clay minerals is critical to the affinity of cesium to them. In addition to this result, effect of substitution between magnesium and iron in the octahedral sheet of phlogopite on the affinity will be reported. This study reveals the pecuilarity of biotite with respect to the affinity. Weathering effects and effects of water molecules on the affinity will be discussed.

[1] Mukai *et al*. (2016) *Sci*. *Rep*. **6**, 21543.