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# First-principles study of cesium adsorption to weathered micaceous clay minerals

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A large amount of radioactive nuclides was produced into environment due to the Fukushima Dai-ichi Nuclear Power Plant (FDNPP) accident. Residents near FDNPP were suffering from radioactive cesium and then evacuated, because which has long half-life and is retained by surface soil for long time. The Japanese government has been decontaminating the cesium by removing the surface soil in order to return them to their home. This decontamination method is very effective, but which produces huge amount of waste soil. This becomes another big problem in Fukushima, because it is not easy to find large storage sites. Then effective and economical methods to reduce the volume of the waste soil are needed. However, it has not been invented yet. One of the reasons is lack of knowledge about microscopic process of adsorption/desorption of cesium to/from soil.
It is known that weathered micaceous clay minerals play crucial role on adsorption and retention of cesium. They are expected to have special sorption sites, called frayed edge sites (FESs), which adsorb cesium selectively and irreversibly. Properties of FES have been intensely investigated by experiments. But microscopic details of the adsorption process on FES are still unclear. Because direct observation of the process with current experimental techniques is quite difficult.
We investigated the adsorption of cesium to FES in muscovite, which is a typical micaceous clay mineral, via first-principles calculations (density functional theory). We made a minimal model of FES and evaluate the energy difference before and after cesium adsorption to FES. This is the first numerical modeling of FES. It was shown that FES does adsorb cesium if the weathering of muscovite has been weathered. In addition, we revealed the mechanism of cesium adsorption to FES, which is competition between ion radius of cesium and the degree of weathering. I plan to discuss volume reduction of the waste soil based on our result.

Reference
M. Okumura, H. Nakamura, and M. Machida, Mechanism of Strong Affinity of Clay Minerals to Radioactive Cesium : First-Principles Calculation Study for Adsorption of Cesium at Frayed Edge Sites in Muscovite, Journal of the Physical Society of Japan 82, 033802 (2013).