

## Molecular Dynamics Study of Adsorption States of Cesium Ion in Cement Matrix

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Cs<sup>+</sup> ion is one of radioactive species generated by nuclear electric power. It is one of the most problematic ions because of its long half-life and high mobility. Cement material is considered as a candidate for the solid fixation of Cs<sup>+</sup> ions, and the engineered barrier for the geological disposal of such radioactive species. The structures of the cement is complicated, and considered as nano-crystalline aggregation phase with two distinct principal local structures, tobermorite and jennite, by the difference of silica-chain length. The goal of this research is to detect which structural or compositional feature is essential to ionic adsorption into cement matrix. By using molecular dynamics simulations, we have studied the aqueous solution-mineral (cement) interfacial systems for two different cement local structures (tobermorite and jennite) and two different solutions (NaCl and CsCl). It was found that Na<sup>+</sup> ion could form both inner-sphere complex and outer-sphere complex, without full hydration shell and with full hydration shell at the time of adsorption, respectively. In contrast, Cs<sup>+</sup> ion could only form inner-sphere complex for both mineral cases. Furthermore, it was found that tobermorite presents better binding property than that of jennite. The fact that differences in cement structure and ion species may cause these differences in adsorption state and binding property will enhance our understanding on cement materials in the case of the solid fixation and the geological disposal.

Keywords: Geological Disposal, Cs Fixation, Ionic Adsorption, Molecular Dynamics