# Estimation of the Enrichment of Cs in Molten Chloride and Fluoride Systems by Molecular Dynamics Simulation

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For the pyrochemical reprocessing of spent metallic fuels in molten salt baths it is of importance to estimate the enrichment degree of Cs. A molecular dynamics simulation has been executed on molten (Li, Na, Cs)Cl at 900 K and (Li, Na, Cs)F at 925 K for various compositions in order to calculate the relative differences in the internal cation mobilities of Cs in molten LiCl-NaCl equimolar mixtures and the LiF-NaF eutectic. According to these results the self-exchange velocities of $Li^+$, $Na^+$ and $Cs^+$ with respect to $Cl^-$ and $F^-$ have similar tendencies at each composition, and Cs can be enriched effectively up to $x_{Cs}$ = 0.5 - 0.6 in LiCl-NaCl melts. In addition, the sequence of the calculated self-diffusion coefficients for various compositions was in a fair agreement with that of the obtained self-exchange velocities.

*Key words:* Molten Ternary Fluorides; Molecular Dynamics Simulation; Internal Cation Mobility; Self-exchange Velocity; Self-diffusion Coefficient.