# Molecular Dynamics Study on the Adsorption Selectivity for Negative Elements in Aluminosilicates

Masahiko Matsumiya and Ryuzo Takagi[a]
Matsumiya Computational Chemistry Institute,
6-14 higashi-numa, machiya-aza, chiaki-cho, ichinomiya-shi, Aichi 491-0813 Japan
[a] Research Laboratory for Nuclear Reactors, Tokyo Institute of Technology,
O-okayama, Meguro-ku, Tokyo 152-8550 Japan

Reprint requests to Prof. M. M.; Fax: 81 586-76-6473; E-mail: molten@d9.dion.ne.jp

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For the pyrochemical reprocessing of spent metallic nuclear fuels in molten salt baths it is important to investigate the adsorption selectivity of cations in aluminosilicates. A molecular dynamics simulation has been performed on sodalite and zeolite with exchangeable monovalent and multivalent cationic fission products at 673 K in order to calculate their self-diffusion coefficients in the aluminosilicate framework and estimate the selectivity of the exchangeable cations. The results enables us to conclude that the self-diffusion coefficients of monovalent cations decrease with increasing ionic radius. The order of the adsorption selectivity is Li < K < Na < Cs in sodalite and Li < Na < K < Cs in zeolite. The self-diffusion coefficients of multivalent cations are almost independent of the ionic radius, and these cations are in aluminosilicates more stable than monovalent cations. The results are consistent with the experimental results.

*Key words:* Adsorption Selectivity; Aluminosilicates Framework; Molecular Dynamics Simulation; Negative Elements; Self-diffusion Coefficient; Sodalite; Zeolite.