Fluorite Ceramic Waste Forms for Actinide Immobilisation

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Fluorite related ceramic materials have attracted considerable attention as potential host materials for the immobilisation of fission products. Research has been carried out into both irradiation damage effects and into the accommodation of fission product ions. Here we have use computer simulations to predict the relative solution energies for Pu and U in 3+ and 4+ charge states ions in $A_2B_2O_7$ pyrochlore compounds. We find that Pu^{3+} is always accommodated at the A site. Pu^{4+} ions are accommodated on both the A and B sites until the ionic radius of the A site cation is below 1Å whereupon it preferentially resides only on the A sites. U^{4+} ions predominantly reside on the B site except when the A site cation radius falls 0.95Å when the A site is preferred.