Diffusion Mechanism of Pu+3 in Sedimentary Repository Conditions: Ab Initio Molecular Dynamics Study

Barbera, Becca (School: Cathedral High School)

The purpose of this experiment was to determine the diffusion coefficient of Pu+3 through MX-80 clay, alongside the interference of the SR-270-PW brine solution of sedimentary rock formations. Using Materials Studio, a molecular dynamic simulation program, a montmorillonite (MMT) unit cell was constructed, then optimized using DMol3 module's GGA-PBE functional. A Pu+3 ion was optimized following the same process. CLAYFF force field parameters were assigned to each atom, then the structure was replicated to form a 1x2x1 supercell, and the C lattice was extended to 18.8Å. 30 H20 molecules and 2 Na+ ions were inserted, then three preliminary simulations, at temperatures of 100K, 200K and 298K, were performed using Forcite dynamics calculations, NPT ensemble, Andersen thermostat and Berendsen barostat. This was followed by an NVT ensemble at 298K simulation. The Pu+3 was then inserted in place of an H2O, and the interlayer model was re-optimized. To mimic the 6.0M Na-Ca-Cl brine solution (SR-270-PW), the appropriate ions were inserted into the water layer, and the structure was reoptimized. Production simulations were conducted using the Forcite module, NVT ensemble, and Nosé thermostat at 298K. Convergence occurred after 14 simulations. The mean squared displacement (MSD) of each individual simulation was calculated, then an average MSD of all the simulations was determined, followed by a linear regression analysis. Using the Einstein relation, $D=\langle|r(t)-r(0)|\rangle/2nt$, the diffusion coefficient of Pu+3, was calculated to be 1.31 ± 0.29 x10-11 m2/s. This study has many valuable applications and provides nuclear waste management organizations with specific data regarding location and storage methods, which will both ensure public protection and support clean-energy production.

Awards Won:

Third Award of $1,000

American Chemical Society: Fourth Award of $1,000