"Plutonium Speciation as Determined by Molecular Modeling"

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We have applied Ab Initio (first principles) MO (molecular orbital) theory to understand Pu speciation in environmental systems. The research is part of a new focus within the National Institute of Standards and Technology to develop Standard Reference Materials that are certified for radionuclide speciation. Our initial attempts have focused on the geometry and energetics of Pu hydrolysis. Reaction simulations were carried out using either Gaussian 94 or 98 (which include spin-orbital functions for actinide elements.) Since Ab Initio calculations are expensive computationally, most calculations were done on NIST's supercomputing systems. (CRAY C90 and IBM SP2 supercomputers). Working with actinides in this way is relatively new and models, when completed, could prove to be useful for determining bioavailability and mobility of actinide complexes. Since many of these species are radioactive and potentially harmful, accurate models could help reduce health hazards.