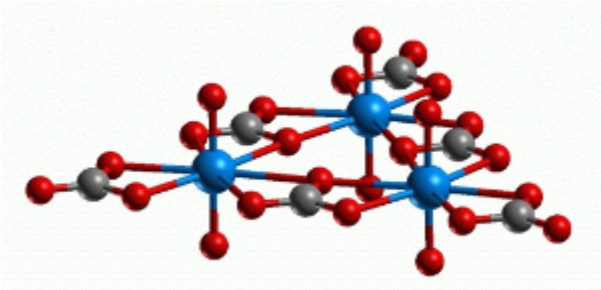
Environmental chemistry of actinides



Complexation of actinides by humic substances is an important topic in environmental science and nuclear waste management. However, the interaction of solvated actinide species with the surfaces of minerals is hardly understood at the atomic level. Our group develops quantum chemistry models of solvated mineral surfaces, focusing on clay minerals as widely available materials. These models are then applied to simulate the sorption of actinide species and other solvated complexes, targeting structure and stability of sorbed complexes with the help of modern DFT methods as well as atomistic-scale simulations.

Our group investigates thermochemical properties of actinide species, such as reaction energies, heats of formation and hydration - all of which are directly related to practical applications. Within the framework of this project, we develop computational methods for the evaluation of key thermodynamic properties of actinide compounds. Recent examples are calculations of the heat of formation of AnO_2^{2+} dications (An = U, Pu).

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