The aim of this project is to develop a robust, efficient and accurate quantum chemical technique for studying the actinide complexes in solvation phase. Actinides (^{89}Ac-^{103} Lr) present a fascinating area of research with their coordination ability, catalytic properties, and unusual bonding schemes. They have specially gained immense importance in recent times due to the fast expanding nuclear power sector. Quantum mechanical studies provide access to the electronic properties of molecules or complexes of these elements as systematic experimental studies with them are constrained by their radioactivity. However, a full quantum mechanics based treatment of the solvated actinide complexes is out of bound due to the restrictive computational demands of such huge systems. Thus, a new hybrid approach will be developed where the actinide complexes will be treated with pair coupled cluster doubles (pCCD) method and the solvent environment will be modeled with effective fragment potential (EFP). The multireference character prevalent in the wave function of actinide molecules restricts the use of standard quantum chemical methods. pCCD has been extensively used for actinides in recent years and has produced highly accurate results for them in gas phase. On the other hand, EFP is a recently developed solvation model where solvent molecules are considered explicitly but their computational burden is replaced by simple preparatory ab initio calculations. Here, each solute molecule is represented by a model potential calculated by taking into account the electrostatic, polarization, dispersion, and exchange-repulsion interactions with all other chemical specie present in the system. Especially, the polarization interaction will be calculated in a self consistent fashion, vastly improving the depiction of solvatochromic effects in the solutions with actinide complexes, which, till now have been mostly studied with dielectric continuum models of solvation. In this project, the theoretical framework of pCCD-EFP method will be designed and implemented in the PyBEST software package. The method will be extended to electronic excited states, where the solvent potentials will be recalculated in response to electron rearrangement due to electronic excitations. The coupling of pCCD and EFP will provide much needed path for accurate investigation of electronic structure, ligation, photochemical processes of actinide complexes in various solvents. Specifically, the developed method will be used to study the aqueous solutions of actinyl compounds ($\mathrm{AnO_2^{n+}}$), building blocks of numerous important components in the nuclear fuel cycle. These studies will directly lead to efficient design of nuclear waste management and sensors for detection of nuclear contamination.