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Theoretical studies of orbital mixing in actinide-ligand bonds

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For the past few years we have put a significant amount of effort into the development of reliable computational methodologies for quantifying the amount of covalent interactions in actinide-ligand bonds. These studies aided the interpretation of ligand core-level spectroscopy measurements by some members of the team and the two efforts together yielded solid evidence of covalent bonding and 5f participation in that interaction. On a more applied side, our studies have been instrumental in elucidating fundamental differences in electronic structure that lead to stronger bonds and selectivity in chemical separations of actinides. In this lecture we will discuss the computational methodologies and the application at prediction of XAS spectra in actinide species. As a corollary we will also discuss the connection between the covalent nature of the bonds and the strength of the bond, which is a concept that has confused the community for a long time. An implicit misunderstanding has been the connection between this evidence of covalent interaction and the relative strength of these bonds. In this presentation we address that issue with quantum mechanical methods to try to clarify and separate the two concepts. These developments are illustrated in a series of molecular complexes where the bonds are clearly defined and described in "simple"language.

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