**Relativistic ab initio Studies of Uranyl and Neptunyl Cations**

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**Abstract**

This poster will present preliminary data in a study on the electronic structure of the uranyl and neptunyl cations and halogenated derivatives. Uranyl is the most abundant form of uranium in the aqueous phase, and has a straightforward geometry and a relatively complicated electronic structure. There are two axial sites available for the species to bond with aqueous ligands, and thus a wide range of interactions are possible between uranyl and other aqueous species.