Abstract Submitted
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Electron binding energy of uranium-ligand and uranyl-ligand anions[1] LEI WANG, STEVEN HOROWITZ, BRAD MARSTON, Brown University — Electron binding energies of the early actinide element uranium in gas-phase anion complexes are calculated by relativistic density functional theory (DFT) with two different exchange-correlation functions (RPBE and B3LYP) and also in the Hartree-Fock (HF) approximation[2]. Scalar and spin-orbit calculations are performed, and the calculated energies are compared to available experimental measurements and shown to disagree by energies of order 1 eV. Strong correlations that are poorly treated in DFT and HF can be included by a hybrid approach in which a generalized Anderson impurity model is numerically diagonalized. Reduction-oxidation (redox) potentials of aqueous actinide ions show improved agreement with measured values in the hybrid approach[3]. We test whether or not similar improvements are found in the gas-phase.

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[2]ADF2010.02, SCM.com
[3]S. E. Horowitz and J. B. Marston, J. Chem. Phys **134** 064510 (2011).

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