Abstract Submitted
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Role of Strong Correlations in Disproportionation of Aqueous Actinides[1] STEVEN E. HOROWITZ, J.B. MARSTON, Brown University — We study the role of strong electronic correlations in the disproportionation of aqueous actinide complexes An(aq) and AnO_2(aq) where An = U, Np, and Pu. Correlations are expected to be important due to the localized nature of the actinide 5f orbitals. We first confirm that relativisitic DFT[2], despite yielding reasonable geometries and bond lengths, fails to reproduce[3] experimentally observed degeneracies of the redox potentials[4]. By using a continuum model for the water beyond the first solvation sphere we are able to construct and diagonalize reduced Hubbard-like models of the actinide complexes, and incorporate the missing physics of strong intra-atomic Coulomb repulsion[5] [6].

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