# DENSITY FUNCTIONAL THEORY CALCULATION OF EXCITED-STATE PROPERTIES OF ACTINIDES

ZHIYONG ZHANG, ROBERT J. HARRISON, *P.O.Box 999, MS K1-83, Richland, WA99352*.

Ground- and excited-state geometres and vibrational frequencies of $UO_2Cl_4^{2-}$ are obtained by DFT calculations. Various approximate functionals are tested and the results are compared with experimental values. The effect of the spin-orbit interaction on the vibrational frequencies is also studied.