EVALUATION OF RELATIVISTIC QUANTUM CHEMISTRY CALCULATIONS THROUGH STUDIES OF URANIUM OXIDES

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Electronic spectra for gas phase UO, UO^+, UO_2 and $UO_2{}^+$ have been recorded recently, and work is continuing on the dioxides. The lowest energy electronic configurations for all of these species include unpaired electrons in the metal 5f orbitals. Consequently, they possess many low-lying electronic states. Prediction of the energy ordering for these states poses a significant challenge for relativistic quantum chemistry calculations. In this presentation we examine the progress that has been achieved in calculating the electronic structures of the oxides and discuss unresolved problems in the interpretation of the data for UO_2. In addition, we will discuss the conflicting evidence concerning the existence of an incipient chemical between UO_2 and Ar.