THEORETICAL CALCULATIONS FOR THE EXCITED STATES AT THE OXYGEN K-EDGE FOR $Cs_2UO_2Cl_4$

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The soft X-ray spectrum of Denning and co-workers (to be published) for the high-lying excited levels at the oxygen K-edge for $Cs_2UO_2Cl_4$ is studied theoretically in an effort to explain the nature of the excited levels. In order to gain some insight into the physical nature of the ionization process, both localized and delocalized hole-state calculations were performed. The single-excitation configuration-interaction results show that the states in the localized hole case are 8-9 eV lower than the corresponding states obtained with the delocalization of the hole onto the two oxygen atoms. The theoretical calculations were also performed with and without the chloride ions in order to study their effect on the Rydberg and valence excited states. A 68-electron relativistic effective core potential was used on the uranium atom. Correlation-consistent polarized double-zeta basis sets were used to perform the calculations.