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High Momentum Transfer Shallow Core-to-valence Spectroscopy in the Actinides SUBHRA SEN GUPTA, Physics Dept., Univ. of British Columbia, Vancouver, Canada, J. A. BRADLEY, Physics Dept., Univ. of Washington, Seattle, USA, M. W. HAVERKORT, Max Planck Inst. for Solid State Research, Stuttgart, Germany, G. T. SEIDLER, Physics Dept., Univ. of Washington, Seattle, USA, G. A. SAWATZKY, Physics Dept., Univ. of British Columbia, Vancouver, Canada — We calculate the dynamic structure factor $S(q,\omega)$ within a renormalized atomic multiplet approach, to describe the 5d→5f non-resonant inelastic x-ray scattering (NIXS) in actinide compounds ThO_2 ($5f^0$) and UO_2 ($5f^2$). For small q, the spectra select the dipole-allowed transitions which are degenerate with continuum states, hindering their use in ground electronic structure determination. However dipole-forbidden multiplets reached with large q are strongly bound to the core-hole, enabling the use of a renormalized atom approach to extract the ground state electronic structure. This crossover from unbound to bound states, reachable by low-q and high-q experiments respectively, is a result of the large multiplet spread of the $5d^9 5f^{N+1}$ multiplets exceeding the attractive core-hole potential. We discuss the details of the calculations and emphasize the importance of high-q experiments in studies of the ground state electronic structure of actinides.

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