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Photoionization of free and confined Mg : Evolution of the cross section with depth of the confining well[1] P. PADUKKA, H.-L. ZHOU, S.T. MANSON, Georgia State University — The photoionization cross sections of the outer $3s^2$ shell of free and confined Mg have been calculated. The C_{60} confinement is modeled as an attractive spherical potential of inner radius 5.8 a.u., thickness of 1.89 a.u. and a depth U_0 varying from 0.0 to 0.302 a.u. (corresponding to Mg@C_{60}). Modified MCHF and HF codes have been used to obtain the single and multi-configuration wave functions, which were calculated self-consistently including the extra confining potential. The photoionization cross sections were calculated using the R-matrix method at both the LS coupling and Breit-Pauli (BP) approximation level. We found that the ionization energy of the Mg ground state increases somewhat with increasing well depth. Moreover the photoionization cross section of free Mg, which is dominated in the threshold region by doubly-excited $nln'l'$ resonances, changes dramatically in the presence of the confining well; partially because many of the near-threshold resonances move below threshold with increasing well depth. In addition the BP calculation shows spin-orbit splitting, significant even at such low Z.

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