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Inner-Shell 2p Photoionization of Free and Confined Mg: Evolution of the Resonances with Depth of the Confining Potential PRABHA PADUKKA, HSIAO-LING ZHOU, STEVEN T. MANSON, Georgia State University — Relativistic Breit-Pauli R-Matrix calculations [1] of the photoionization cross sections of the inner 2p shell of free Mg and Mg confined in a C₆₀ molecule have been performed. The C₆₀ confinement potential is modeled as an attractive spherical potential of inner radius 5.8 a.u., thickness of 1.89 a.u. and a depth U₀ of 0.302 a.u. Multi-configuration wave functions for the final states of the ion core (target states) were obtained using modified MCHF and HF codes [2]. The calculations were performed for a variety of well depths up to 0.302 a.u in order to study the evolution of the photoionization cross section from free Mg to Mg@C₆₀. Particular attention was paid to the autoionizing resonances arising from the excitation 2p_{1/2} and 2p_{3/2}; the lowest five series are given as 2p⁵(²P_{3/2})ns[3/2], 2p⁵(²P_{1/2})ns[1/2], 2p⁵(²P_{3/2})nd[3/2], 2p⁵(²P_{3/2})nd[1/2], 2p⁵(²P_{1/2})nd[3/2]. The resonances were identified and characterized using the eigenphase derivative technique, the QB method [3], and quantum defect theory. A complex pattern of changes occur with increasing well depth, with some of the resonances moving to lower photon energy and some to higher. This behavior is explained in terms of how the discrete orbitals are altered by the increasing depth of the well. [1] K. A. Berrington, W. B. Eissner, and P. H. Norrington, *Comput. Phys. Commun.* **92**, 290 (1995); [2] C. Froese Fischer, *Comput. Phys. Commun.* **64**, 431 (1991); [3] L. Quigley and K. Berrington, *J. Phys. B* **29**, 4529 (1996).

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