

Relativistic R-matrix calculation photoionization cross section of Xe and Xe@C₆₀

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The properties and behavior of endohedral fullerenes A@C₆₀, where atom A is encapsulated inside the interior of a fullerene cage, have gained considerable interest in physics, chemistry, material science and nanoscience in recent years (see review papers [1-2], and references therein). An effective method to study such confined atoms is photoionization. Confinement resonances produced in the photoionization of Xe@C₆₀ have been demonstrated in the notable breakthrough experiment by Kilcoyne and Co-workers [3]. Meanwhile, a number of theoretical calculations have been carried out using different methods. In the present work, the atomic structure of Xe and Xe@C₆₀ are studied using the multiconfiguration Dirac-Fock (MCDF) method, and the photoionization cross sections are calculated using the fully relativistic R-matrix method [4]. The C₆₀ fullerene cage has been commonly modeled as a spherical attractive cavity and more recently with a newly proposed jellium model [5]. Comparison between the present calculations and other experimental and theoretical results demonstrate that configuration interaction plays an important role. The resonance profile resulting from confinement by the fullerene cage compares well with experimental measurements [3].

References:

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