Photoionization of Ce$^{3+}$@C$_{82}$$^1$ ZHIFAN CHEN, ALFRED Z. MSEZANE, Clark Atlanta University — Photoionization cross section for the Ce$^{3+}$@C$_{82}$ endohedral fullerene in the energy region 100-150 eV has been studied using our open-shell random phase approximation with exchange method and the C$_{82}$ model potential. Electron affinity (EA) of the C$_{82}$ has been calculated using the density functional theory. The C$_{82}$ fullerene was described by an attractive short range spherical well with potential $V(r)$, given by $V(r) = -V_0$ for $r_i < r < r_0$, otherwise $V(r) = 0$. $V_0$ was obtained by solving the resultant transcendental equation using the calculated EA value. The wave functions of the Ce$^{3+}$ confined inside the C$_{82}$ have been calculated by solving the Schrödinger equation with both regular and irregular solutions and the continuous boundary conditions of the wave functions and their logarithmic derivatives at $r_i$ and $r_0$. Our calculation included 32 ionization channels from 5s, 5p and 4f subshells and 14 channels from the $4d^{10}\ 4f^2 +h\nu \rightarrow 4d^{9}4f^2$ photoexcitation. Finally the RPAE equation was solved to obtain the partial cross sections with a total of 16 $^2$D states, 16 $^2$G states and 14 $^2$F states. The photoionization of Ce$^{3+}$@C$_{82}$ shows both the resonance and suppression effect and demonstrates a more stronger resonance peak at 106 eV.

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