

Abstract Submitted  
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**Photoionization of  $Ce^{3+}@C_{82}$** <sup>1</sup> 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  $4d^{10} 4f + h\nu \rightarrow 4d^9 4f^2$  photoexcitation. Finally the RPAE equation was solved to obtain the partial cross sections with a total of 16  $^2D$  states, 16  $^2G$  states and 14  $^2F$  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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