Suppression of the 4d resonance single-photoionization of $Ce@C_{82}^{+}$

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We investigate the single-photoabsorption spectrum for endohedral cerium in $Ce@C_{82}^{+}$. The fullerene cage is modelled by a spherical "jellium-shell" [1,2]. To explain the fact of suppression of photoionization cross section observed experimentally by Müller et al. [3] we consider the corresponding Auger $4d^{-1}$ decay from the cerium free ion Ce^{3+} and the ion $Ce^{3+@}$ encapsulated in $Ce@C_{82}^{+}$ (in practice, $Ce^{3+}@C_{82}^{2-}$). We calculate the oscillator strength within the resonance region (100-160 eV) for phototransition from outermost shells of ion Ce^{3+} and encapsulated ion $Ce^{+3@}$ within the Multiconfiguration Dirac-Fock(MCDF) method with and without account for influence of the potential generated by the fullerene cage. It is shown that the oscillator strengths have the main contribution from the Ce^{3+} "$4d \rightarrow 4f$" resonance photoexcitations. Our calculations demonstrate that the oscillator strengths $f_{4d \rightarrow 4f}$ are affected (decreased) very slightly by including of the cage potential. We present the photoabsorption cross section calculated with the cage potential taken into account and with no account for it taken. The Lorenzial profiles are presented. It is shown that the main reason of changing in the absorption cross section curve (decreasing of the maximum values), and the corresponding decrease of integrated oscillator strength values, is the increasing in Auger transition line widths (that are calculated within MCDF) due to interaction of photoelectrons with cage electrons. The reduction of the integrated oscillator strength is demonstrated. Our results can be compared with the recent measurements by Müller et al. [3].

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Inner-shell photoionisation of fullerenes C_{20} and C_{60}. High-energy cross section assymptotics.

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The nearly spherical cage form of carbon clusters such as fullerenes C_{60} (I_h) and C_{20} (C_2 or C_i point groups) in the first approximation might be considered as a spherical bubble. Then the potential energy is modeled by a spherical delta-function ("Dirac bubble") potential $V(r)= -A\delta(r-R)$, where A is the strength parameter, R is the fullerene radius. The quantum mechanical problem was considered by Blinder (1979) [1] by exploiting isomorphisms with free-particle partial-wave Green function. Until now the deltafunction model was applied only to description of an electron, bound or detached, in the field of neutral C_{60} molecules, i.e. negative fullerene ions C_{60}^{-}[2]. The goal of the present work is to investigate the photoionisation by high-energy photons (1-3 au) from the inner shells (1s and 2p) of the valence band of the fullerenes C_{60} and C_{20}. The whole energy spectra of σ (according to the terminology usually used for modeling the planar graphite surface) orbitals and behavior of corresponding wave functions calculated within our model with the proper choice of strength parameter values A are in good agreement with the other theoretical results for $C_{60}$and C_{20} systems obtained by Ivanov et al.[3] and by Gianturco et al.[4], respectively.

Photoelectron (continuum) wave functions are specified in terms of phase shifts and normalizations. The partial cross sections are calculated (numerically in the length gauge and analytically in the acceleration gauge). This allows us to discuss the presence of resonances (shape resonances), which will cause the structure features in cross sections. We analyze phaseshift behaviour for s-, p-, d- partial waves which is of oscillation type and corresponding partial and total cross sections. As result, the total cross sections reveal an iteresting "serrated" structure.

High-energy cross section asymptotics is deduced (k is an electron momentum, ω is a photon energy) - it is inverse 5/2 power fall off in energy, modulated by oscillating trig functions: $\sigma \sim \omega^{-5/2} \sin^2 (kR)$.

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