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Corrigendum: Diffuse versus square-well confining potentials in modelling $A@C_{60}$ atoms (2012 *J. Phys. B: At. Mol. Opt. Phys.* **45** 105102)

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A factor '2' in both terms on the right-hand-side of equation (2) on page 2 in the original article was the authors' typo in write-up and must be discarded as such. The correct equation (2) reads as follows:

$$U_{\mathrm{DP}}(r) = \left.\frac{U_0}{1+\exp\left(\dfrac{R_0-r}{\eta}\right)}\right|_{r\leqslant R_0+\frac{1}{2}\Delta} + \left.\frac{U_0}{1+\exp\left(\dfrac{r-R_0-\Delta}{\eta}\right)}\right|_{r>R_0+\frac{1}{2}\Delta}. \qquad (2)$$

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Diffuse versus square-well confining potentials in modelling $A@C_{60}$ atoms

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Abstract

A perceived advantage for the replacement of a discontinuous square-well pseudo-potential, which is often used by various researchers as an approximation to the actual C_{60} cage potential in calculations of endohedral atoms $A@C_{60}$, by a more realistic diffuse potential is explored. The photoionization of endohedral $H@C_{60}$ and $Xe@C_{60}$ is chosen as the case study. The diffuse potential is modelled by a combination of two Woods–Saxon potentials. It is demonstrated that photoionization spectra of $A@C_{60}$ atoms are largely insensitive to the degree η of diffuseness of the potential borders, in a reasonably broad range of ηs. These spectra are found to be insensitive to discontinuity of the square-well potential as well. Both potentials result in practically identical calculated spectra. New numerical values for the set of square-well parameters, which lead to a better agreement between experimental and theoretical data for $A@C_{60}$ spectra, are recommended for future studies.

(Some figures may appear in colour only in the online journal)

1. Introduction

Photoionization of atoms A encapsulated inside the hollow interior of the C_{60} fullerene cage, labelled as $A@C_{60}$ and referred to as endohedral or confined atoms, has been an *ad hoc* topic of numerous theoretical (see review papers [1, 2] and references therein in addition to other references in the present paper) and experimental [3] (and references therein) studies in recent years. A theory of $A@C_{60}$ photoionization, based on first principles, has not been developed yet, in view of the formidable complexity of the problem. Perhaps, the most sophisticated theory here is represented by a time-dependent local density approximation (TDLDA), see, e.g., [4] and references therein. However, the current TDLDA theory has obvious drawbacks in view of an unsatisfactory agreement with the existing experimental data on the $Xe@C_{60}^{+}$ 4d photoionization [3]. Meanwhile, many important insights into the problem can be, and have been, unravelled on the basis of simpler empirical models based on the modelling of C_{60} confinement by pseudo-potentials, such as a δ-function-like potential [5, 6] (and references therein) or square-well potential, $U_{SWP}(r)$. The latter is defined as

$$U_{SWP}(r) = \begin{cases} -U_0, & \text{if } R_0 \leqslant r \leqslant R_0 + \Delta \\ 0 & \text{otherwise.} \end{cases} \quad (1)$$

Here, R_0 is the inner radius of C_{60}, Δ is the thickness of the C_{60} wall and U_0 is the potential depth. The square-well potential modelling of C_{60} has become quite popular among various researchers. It has been used on numerous occasions in the field of C_{60} and $A@C_{60}$ theoretical studies, see, e.g., [1, 2, 7–19] and references therein.

The potential $U_{SWP}(r)$, however, is discontinuous at its borders. A possible emergence of qualitative and, especially, quantitative artefacts in calculated $A@C_{60}$ spectra, due to said discontinuity, in calculated photoionization cross sections has not been detailed in the literature except for a couple of brief remarks made on the subject in passing [20, 21]. In particular, it is because of the lack of such knowledge that it has recently been proposed [22] to replace the square-well potential modelling of the C_{60} by a smooth Gaussian-function-like model potential. However, the latter continuously changes strongly everywhere inside the C_{60} cage, thereby having no compact borders. This contradicts a recent Fourier imaging study of the experimental C_{60} photoionization cross section [23]. The study shows that C_{60} has well-defined, compact borders. In short, following the logic line of [20, 23], photoionization of an atomic cluster occurs with the greatest probability where the cluster's potential changes sharply. This is obvious from the acceleration form gauge for a dipole

photoionization amplitude, D, namely $D \propto (\psi_f|\Delta_r V(r)|\psi_i)$. Based on this, it was determined [23] that C_{60} has sharp borders rather than soft borders. Correspondingly, the assumption for a Gaussian-function-like potential of C_{60} is incorrect.

Surely, a C_{60} confining potential with diffuse (rounded) but compact borders, if defined appropriately, is more realistic than a square-well potential with infinitely sharp edges. However, it is not at all clear beforehand to what degree replacement of the square-well potential for a diffuse potential may improve or worsen agreement between experiment and theory. The need for clarifying this issue is signified by the fact that the square-well potential modelling of $A@C_{60}$ atoms has been used abundantly over the years. This has resulted in a large array of predicted data and phenomena that might need to be restudied/recalculated with an eye on more realistic diffuse potential borders. It is the aim of this paper to dot *i*s and cross *t*s regarding the stated concerns.

To attain the aim, we calculate the photoionization cross sections of, and photoelectron angular distribution from, inner and valence subshells of $A@C_{60}$ atoms by utilizing both $U_{\rm SWP}(r)$ and $U_{\rm DP}(r)$ as the C_{60} confining potentials. As a result, we find that discontinuity of the $U_{\rm SWP}(r)$ potential leads neither to qualitative nor quantitative artefacts in calculated photoionization characteristics of $A@C_{60}$ atoms compared to calculated data obtained with the use of the diffuse potential $U_{\rm DP}(r)$. Moreover, it is found that the degree of diffuseness of the $U_{\rm DP}(r)$ potential matters surprisingly little—a fraction-to-nothing—in a relatively broad range of its values.

Atomic units (au) are used throughout this paper.

2. Theory, results and discussion

2.1. Review of theory

In this work, a square-well potential $U_{\rm SWP}(r)$ is given by (1). As for a diffuse potential $U_{\rm DP}(r)$, it is defined by a combination of two Woods–Saxon potentials:

$$U_{\rm DP}(r) = \left.\frac{2U_0}{1+\exp\left(\frac{R_0-r}{\eta}\right)}\right|_{r\leqslant R_0+\frac{1}{2}\Delta} + \left.\frac{2U_0}{1+\exp\left(\frac{r-R_0-\Delta}{\eta}\right)}\right|_{r>R_0+\frac{1}{2}\Delta}. \quad (2)$$

Here, η is the diffuseness parameter, and R_0, U_0 and Δ are the same as the parameters of the square-well potential.

Concerning photoionization of $A@C_{60}$ atoms, we focus on the photoionization cross section $\sigma_{n\ell}(\omega)$ of a $n\ell$-subshell of $A@C_{60}$ as well as dipole photoelectron angular-asymmetry parameter $\beta_{n\ell}(\omega)$. For free atoms, they are determined by equations presented, e.g., in [24, 25]. The latter are equally applicable to endohedral atoms $A@C_{60}$ as well, in our modelling of such atoms. Correspondingly,

$$\sigma_{n\ell} = \frac{4\pi^2\alpha N_{n\ell}}{3(2\ell+1)}\omega[\ell|D_{\ell-1}|^2 + (\ell+1)|D_{\ell+1}|^2], \quad (3)$$

and we prefer to recast $\beta_{n\ell}(\omega)$ as

$$\beta_{n\ell} = \frac{\ell(\ell-1)\rho^2 - 6\ell(\ell+1)\rho\cos\Phi + (\ell+1)(\ell+2)}{(2\ell+1)(\rho^2\ell+\ell+1)}. \quad (4)$$

Here,

$$\rho = \frac{|D_{\ell-1}|}{|D_{\ell+1}|}, \quad \Phi = \delta_{\ell+1} - \delta_{\ell-1}. \quad (5)$$

In the above equations, ω is the photon energy, $N_{n\ell}$ is the number of electrons in a $n\ell$ subshell, α is the fine-structure constant, $D_{\ell\pm1}$ are radial dipole photoionization amplitudes and $\delta_{\ell\pm1}$ are phase shifts of $D_{\ell\pm1}$. Note that the quantities $\sigma_{n\ell}$, $\beta_{n\ell}$, $D_{\ell\pm1}$, ρ, $\delta_{l\pm1}$ and Φ all depend upon photon energy ω; the explicit dependence is omitted in the above equations for reasons of simplicity.

In an independent particle approximation, $D_{\ell\pm1}$ is defined as

$$D_{\ell\pm1} = \int_0^\infty P_{\epsilon\ell\pm1}(r) r P_{n\ell}(r)\,{\rm d}r, \quad (6)$$

where $P_{n\ell}(r)$ and $P_{\epsilon\ell}(r)$ are one-electron radial wavefunctions of the bound and continuous states, respectively. In the present work, these wavefunctions and energies $E_{n\ell}$ of a discrete spectrum are the solutions of a modified radial Hartree–Fock (HF) equation accounting for a $U_{C_{60}}(r)$ confinement:

$$[\hat{H}^r + U_{C_{60}}(r)]P_{n\ell}(r) = E_{n(\epsilon)\ell}P_{n(\epsilon)\ell}(r). \quad (7)$$

Here, $\hat{H}^r$ is a radial part of the HF Hamiltonian which is identical to that for a free atom [24], and $U_{C_{60}}(r)$ is either the square-well potential $U_{\rm SWP}(r)$ (1) or diffuse potential $U_{\rm DP}(r)$ (2).

In a particular case of an endohedral single-electron hydrogen atom, $H@C_{60}$, (7) reduces to a radial Schrödinger equation in the presence of the C_{60} confinement:

$$-\frac{1}{2}\frac{{\rm d}^2P_{n(\epsilon)\ell}}{{\rm d}r^2} + \left[\frac{-1}{r} + \frac{\ell(\ell+1)}{2r^2} + U_{C_{60}}(r)\right]P_{n(\epsilon)\ell}(r) = E_{n(\epsilon)\ell}P_{n(\epsilon)\ell}(r). \quad (8)$$

To calculate $D_{\ell\pm1}$ beyond the independent particle HF approximation, i.e. to account for electron correlation, we utilize a random phase approximation with exchange (RPAE) [24].

2.2. Results and discussion

In this work, when approximating the C_{60} potential by a square-well or diffuse potential, we use $U_0 = -0.422$, $\Delta = 1.25$ and $R_0 = 6.01$ au [26] rather than $U_0 = -0.302$, $\Delta = 1.9$ and $R_0 = 5.89$ au used in previous calculations by these and many other authors, see, e.g., [1, 2, 13]. This is because the new parameters were shown [26] to result in a much better match of calculated photoionization spectra to experimental

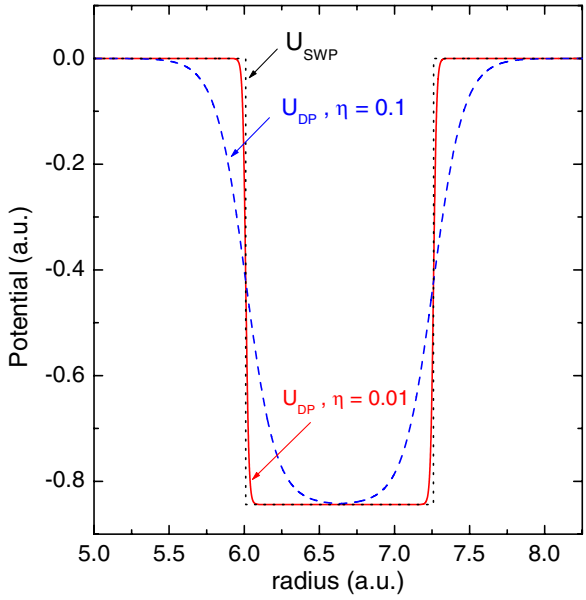

Figure 1. The square-well potential $U_{\rm SWP}(r)$ (1) with $U_0 = -0.422$, $\Delta = 1.25$ and $R_0 = 6.01$ au (dotted line), as well as the diffuse potential $U_{\rm DP}(r)$ (2) with the diffuseness parameter $\eta = 0.01$ (solid line) and $\eta = 0.1$ (dashed line). See text for details.

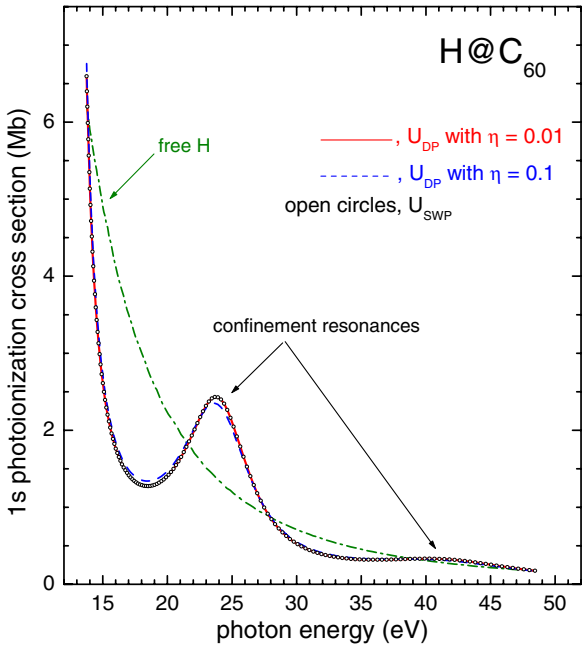

Figure 2. Hydrogen 1s photoionization cross section of H@C_{60} calculated with the use of the square-well potential $U_{\rm SWP}(r)$ (open circles), diffuse potential $U_{\rm DP}(r)$ with $\eta = 0.01$ (solid line) and $\eta = 0.1$ (dashed line), and of free hydrogen, as marked.

spectra of endohedral atoms, particularly the 4d spectrum of Xe@C_{60}^+ [3].

Calculated data for thus defined $U_{\rm SWP}(r)$ and $U_{\rm DP}(r)$ are compared with each other in figure 1 for two different values of the diffuseness parameter η of $U_{\rm DP}(r)$, namely $\eta = 0.01$ and 0.1 . One can see from figure 1 that $U_{\rm DP}(r)$ with $\eta = 0.01$ and the square-well potential are practically identical. In contrast, for $\eta = 0.1$, calculated $U_{\rm DP}(r)$ has strongly diffuse borders, thereby noticeably deviating from the square-well potential.

In the following, we detail results of comparison between $\sigma_{n\ell}(\omega)$ and $\beta_{n\ell}(\omega)$ calculated with the use of the $U_{\rm SWP}(r)$ and $U_{\rm DP}(r)$ confining potentials.

As the first step, in order to avoid various possible complications due to electron correlation in multielectron atoms, we discuss a 'clean' case—the photoionization of the 1s ground state of the endohedral hydrogen atom, H@C_{60}. Corresponding results are depicted in figure 2.

First, we note that the photoionization cross section $\sigma_{1s}(\omega)$ of H@C_{60}, calculated with the use of a diffuse potential $U_{\rm DP}(r)$ with a small diffuseness parameter $\eta = 0.01$, is practically undistinguishable from $\sigma_{1s}(\omega)$ calculated in the square-well potential modelling of H@C_{60}. Hence, discontinuity of the square-well potential does not result in any artefacts in $\sigma_{1s}(\omega)$. Second, what comes as a big surprise, is that calculated $\sigma_{1s}(\omega)$, obtained with the use of a much greater diffuseness parameter $\eta = 0.1$, is practically identical to $\sigma_{1s}(\omega)$ calculated either with $\eta = 0.01$ or in the framework of the square-well potential model. This suggests that the photoionization of an endohedral atom may be rather insensitive to the degree of diffuseness of the confining potential, in reasonably large limits. As a note on an independent issue, one can see that the photoionization cross section of free hydrogen differs from that of H@C_{60} by the presence of a well-developed maximum at about 25 eV and insignificant maximum at about 41 eV in the cross section. These are called confinement resonances, i.e. resonances that occur due to a constructive interference of the outgoing photoelectron wave and photoelectron waves scattered off the C_{60} cage [1, 2, 5] (and references therein). Confinement resonances have only recently been experimentally proven to exist [3].

Next, we investigate whether the above findings are valid for photoionization of inner shells and valence shells of endohedral multielectron atoms A@C_{60} where electron correlation is strong. To date, only photoionization of endohedral Xe@C_{60}^+ has been reliably measured experimentally [3]. Therefore, we choose photoionization of Xe@C_{60} as the case study to learn how discontinuity of $U_{\rm SWP}(r)$ or diffuseness of $U_{\rm DP}(r)$ may affect photoionization cross sections $\sigma_{n\ell}(\omega)$ of, and photoelectron angular-asymmetry parameters $\beta_{n\ell}(\omega)$ from, the Xe@C_{60} inner $4d^{10}$ and valence $5p^6$ subshells. The comparison of our calculated data for neutral Xe@C_{60} with experimental data for charged Xe@C_{60}^+ [3] is appropriate because [1, 27] charging the C_{60} shell positively does nothing to the photoionization cross section (as a function of photon energy) except to increase the threshold energy. Note, $\beta_{n\ell}(\omega)$ depends on phase shifts $\delta_{\ell\pm1}$ of photoionization matrix elements. Hence, corresponding calculated data will provide, although implicitly, the information on sensitivity of phase shifts $\delta_{\ell\pm1}$ to diffuseness of a confining potential as well. Both HF and RPAE calculated data for $\sigma_{4d}(\omega)$ and $\beta_{4d}(\omega)$, as well as for $\sigma_{5p}(\omega)$ and $\beta_{5p}(\omega)$, are depicted in figures 3 and 4, respectively.

One can see from figures 3 and 4 (compare dashed curves marked as '$U_{\rm SWP}$' with solid curves marked as '$U_{\rm DP}$, $\eta = 0.1$') that calculated data for $\sigma_{n\ell}(\omega)$ and $\beta_{n\ell}(\omega)$, obtained with the

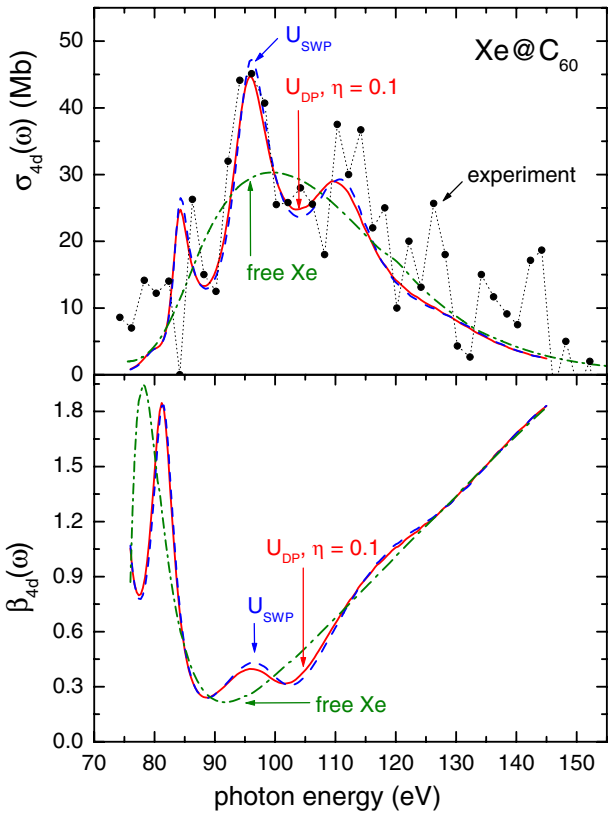

Figure 3. RPAE calculated data for $\sigma_{4d}(\omega)$ and $\beta_{4d}(\omega)$ of Xe@C_{60} obtained with the use of the square-well potential $U_{SWP}(r)$ (dashed lines) and diffuse potential $U_{DP}(r)$ with $\eta = 0.1$ (solid lines), as marked. Also depicted are corresponding RPAE calculated data for free Xe (dashed-dotted lines) and experimental data for $\sigma_{4d}(\omega)$ of Xe@C_{60}^{+} [3]. Experimental data were shifted by 4.2 eV towards higher photon energies as well as multiplied by 10 to compare with theory (see discussion in the appendix).

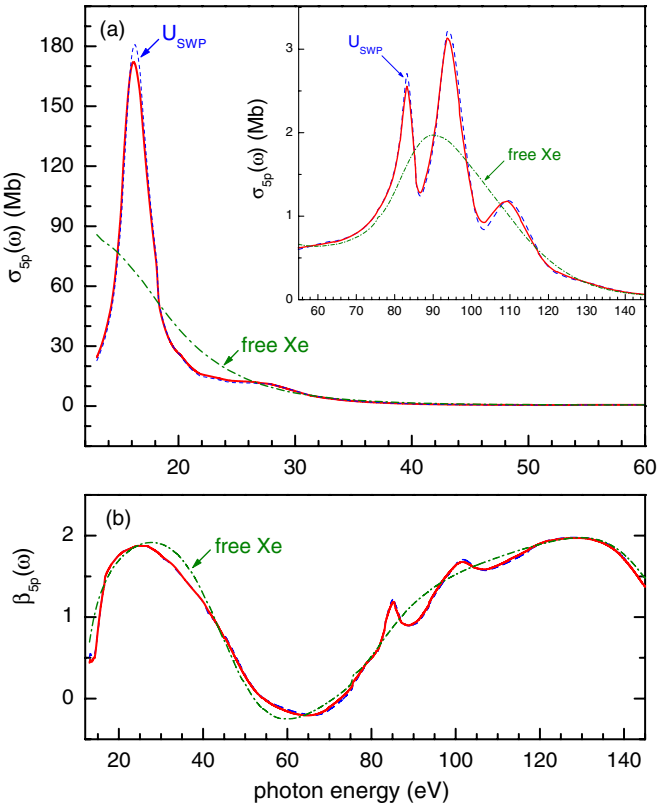

Figure 4. RPAE calculated data for Xe@C_{60} 5p photoionization cross section, $\sigma_{5p}(\omega)$, and dipole photoelectron angular-asymmetry parameter, $\beta_{5p}(\omega)$, calculated with the use of the square-well potential $U_{SWP}(r)$ (dashed lines) and diffuse potential $U_{DP}(r)$ with $\eta = 0.1$ (solid lines). Also depicted are RPAE calculated data for $\sigma_{5p}(\omega)$ and $\beta_{5p}(\omega)$ for free Xe (dashed-dotted lines).

use of either of the two potentials, are practically identical even in the presence of a strong electron correlation in the atom. This leads us to the conclusions outlined in the next section.

3. Conclusion

To summarize, it has been proven in this paper that discontinuity of a square-well potential does not lead to any artefacts, whether quantitative or qualitative, in photoionization spectra of endohedral atoms. The square-well potential modelling of C_{60} is as good as its modelling by a diffuse potential. Both of these potentials lead to practically identical calculated data for photoionization spectra. The latter are largely insensitive to the degree of diffuseness. Hence, both potentials work equally when approximating the C_{60} cage potential. The implication is that replacing the square-well potential by a more realistic diffuse potential, if wanted, will not require a restudy of a rich variety of important results on A@C_{60} ionization phenomena accumulated to date on the basis of the square-well confining potential concept.

Finally, since the values used here of the square-well potential parameters $R_0 = 6.01$, $\Delta = 1.25$ and $U_0 = 0.422$ au result in a reasonable agreement with experiment (see figure 3), we suggest the users of the square-well potential modelling of A@C_{60} to utilize these updated parameters in their future work on the subject.

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Appendix. The 4d and 5p photoionization of Xe@C_{60}

To finalize the paper, we now briefly comment on particular features and structures in the calculated 4d and 5p spectra of Xe@C_{60} depicted in figures 3 and 4, since they are important stand-alone qualities.

To start with, the three strong oscillations in $\sigma_{4d}(\omega)$ of Xe@C_{60} about $\sigma_{4d}(\omega)$ of free Xe are confinement resonances. They were previously theoretically studied and detailed in [4, 5, 15, 13, 26] (and references therein). Experimentally, confinement resonances in A@C_{60} photoionization were observed only recently, in the 4d giant resonance spectrum of Xe@C_{60}^{+}, as the case study [3]. Results of the measurement are by about a factor of 10 smaller than the cited theoretical data. This is because the measured channel of the Xe@C_{60}^{+} 4d

photoionization might account for only about 10% of the Xe 4d oscillator strength [3]. For this reason, to ease the comparison with the theoretical data presented herein, the experimental data were multiplied by 10, and so depicted in figure 3. One can see that calculated results for $\sigma_{4d}(\omega)$ of Xe@C_{60}, obtained with the use of $R_0 = 6.01$, $\Delta = 1.25$ and $U_0 = 0.422$ au, are in reasonable agreement with the main structures of the experimental spectrum, to a good approximation. Of course it would be too naive to expect our simple model to account for all qualitative and quantitative features of the measured Xe@C_{60}^+ photoionization which (the model), among other things, accounts for only a single-electron 4d ionization. Thus, for example, while confinement brought oscillations in the experimental spectrum definitely emerge from the single-electron photoionization, possible double-electron satellites might affect their positions and amplitudes as well. We, however, assume that such contributions are not decisive, so that omitting them, as in the present work, is a reasonable first step towards the initial understanding of the experimental data.

To conclude the discussion on the Xe@C_{60} 4d photoionization we note that, recently, another group of theorists [19] has reported results of their own calculations of the Xe@C_{60} 4d photoionization. They used exactly the same approximations as three other *independent* theoretical groups [15, 13, 28] (i.e. RPAE (or relativistic RPAE [15]) and square-well confining potential with identical parameters). However, results of work [19] differ strongly from results of all of the three cited theoretical groups (the latter are in good agreement with each other). We conclude that something was not right in work [19], most likely because of the very peculiar way those authors chose to solve HF equations in the presence of a square-well potential confinement.

Commenting on $\sigma_{5p}(\omega)$ of Xe@C_{60}, see figure 4(a), we note that a strong maximum at the 5p threshold as well as a less-developed oscillation at about 28 eV in $\sigma_{5p}(\omega)$ are confinement resonances. Interestingly, they are absent in $\beta_{5p}(\omega)$. This is because the 4d $\rightarrow$ f transition absolutely dominates over the 4d $\rightarrow$ p transition at given energies both for free Xe and Xe@C_{60}. Correspondingly, the parameter ρ (5) is negligible, $\rho \ll 1$, in both atoms. As a result, it vanishes from the equation for $\beta_{n\ell}$ (see (4)), and so do the confinement resonances in question. At higher energies, above 70 eV, $\sigma_{5p}(\omega)$ is dominated by three strong resonances. Their positions approximately match the positions of confinement resonances in $\sigma_{4d}(\omega)$, see figure 3. The same situation has recently been found in the Xe@C_{60} 5p generalized oscillator strength [29]. As in [29], the present study reveals that the resonances in $\sigma_{5p}(\omega)$ beyond 70 eV are induced by the confinement resonances in the 4d photoionization channels, via interchannel coupling. Thus, the resonances in $\sigma_{5p}(\omega)$ beyond 70 eV are *correlation* confinement resonances [1, 4, 13, 15, 30]. Correlation confinement resonances in A@C_{60} photoionization are resonances that emerge in the photoionization of an outer subshell due to interference of transitions from the outer subshell (5p in our case) with confinement resonances emerging in *inner* shell transitions (4d transitions in our case), via interchannel coupling. Next, one can see from figure 4(b) that these correlation confinement resonances emerge in $\beta_{5p}(\omega)$ as well, at about 85 and 100 eV. This is because the otherwise dominant 4d $\rightarrow$ f transition is minimized at these energies, as clearly follows from data for $\sigma_{5p}(\omega)$. The amplitudes of 4d $\rightarrow$ f and 4d $\rightarrow$ p transitions become comparable, so that $\rho \sim 1$, in contrast to $\rho \ll 1$ when 4d $\rightarrow$ f is maximized. Correspondingly, the parameter ρ noticeably oscillates through the photon energy region of 70–110 eV, and so does $\beta_{5p}(\omega)$. This is why noticeable confinement resonances emerge in $\beta_{5p}(\omega)$ above 70 eV, in contrast to their absence near threshold. Finally, we note that we ignored the C_{60} plasmon resonance impact [4, 10, 31] (and references therein) on the Xe@C_{60} 5p ionization, although it is known to be significant up to about 70 eV of photon energy. The omission is justified because the primary aim of this paper is to study relative differences between the effects of the diffuse and square-well confining potentials on A@C_{60} photoionization. The C_{60} plasmon resonances cannot alter these differences. For the same reason, we omitted accounting for the existing, but generally weak, interior static-polarization effect in A@C_{60} [32].

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