

Hybridization-related correction to the jellium model for fullerenes

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Abstract. We introduce a new type of correction for a more accurate description of fullerenes within the spherically symmetric jellium model. This correction represents a pseudopotential which originates from the comparison between an accurate *ab initio* calculation and the jellium model calculation. It is shown that such a correction to the jellium model allows one to account, at least partly, for the sp^2 -hybridization of carbon atomic orbitals. Therefore, it may be considered as a more physically meaningful correction as compared with a structureless square-well pseudopotential which has been widely used earlier.

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1. Introduction

Since the discovery of fullerenes by Kroto *et al.* [1] in 1985, these molecules have been the objects of intensive experimental and theoretical investigations (see, e.g., [2]). At present, the investigation of fullerenes is active since they are proposed to be used in various fields of science and technology. For instance, excitation of fullerenes, placed in a biological medium, by an external radiation or incident heavy ions may lead to an active generation of secondary electrons or reactive oxygen species. This allows fullerenes to be potentially used as sensitizers in photodynamic therapy [3]. A very important fundamental problem closely related to the aforementioned application is an adequate description of dynamic response of fullerenes to external fields or to the interaction with projectiles. Processes of scattering of electrons, photons and heavy charged particles on various atomic clusters and fullerenes, in particular, have been actively studied during the past several decades (see, e.g., the review [4] and references therein). Not the least of the factors for a proper description of the dynamic response

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of a many-electron system is an adequate description of the ground- and excited-state (including excitation into continuum) properties of the system under study.

Contemporary software for quantum-chemical calculations (e.g., Gaussian 09 [5]) provides an accurate quantitative description of the ground state of many-particle systems (fullerenes, in particular), and allows one to obtain information on geometrical and chemical properties of the system. However, the description of dynamic properties, which play an important role in the process of photoionization, by means of such programs faces significant difficulties. Dynamic properties (e.g., dynamic polarizability) are closely related to the response of a many-electron system to an external electromagnetic field. In many cases, the properties are governed by a collective excitation of electrons and the formation of plasmon resonances in the excitation spectra [6]. In various systems plasmon resonances lie either below the ionization threshold (in metal clusters) or above it (e.g., in fullerenes). Out of these two classes of atomic clusters, only the optical response of metal clusters has been calculated so far with the help of quantum-chemical programs (see, e.g. [7, 8]). Collective electron excitations in fullerenes, which lie in the continuous spectrum, have not been described so far by means of quantum-chemical programs. However, this can be achieved within simplified model approximations. A minimum requirement is that these approximations must provide an accurate quantitative description of the ground-state features of the systems under study, in order to be applied to the investigation of the dynamic response and to the calculation of the photoabsorption (or, in particular, photoionization) spectrum.

One of the well-known and widely used approaches is based on the jellium model [9]. It was applied frequently to the description of ground-state properties of metal clusters [9–11] and fullerenes [12, 13], as well as to the investigation of photoexcitation processes arising in these systems [13–21].

In [12, 22], it was stated that the ground-state properties of fullerenes cannot be described properly by the standard jellium model which produces, in particular, unreliable values for the total energy [12]. To avoid this, adding of *structureless* pseudopotential corrections was suggested [12]. As a rule, a phenomenological square-well (SW) pseudopotential has been commonly used in the calculations [12, 16, 18, 21]. It was claimed that accounting for such a pseudopotential increases the accuracy of the jellium-based description [16] and, for instance, allows one to reproduce the experimental value of the first ionization potential of C₆₀ [21]. Nonetheless, the applicability of the jellium model for fullerenes and the choice of parameters of the used SW pseudopotential have not been clearly justified so far from a physical viewpoint.

In this paper, we use another methodology and introduce a *structured* pseudopotential which originates from the comparison of an accurate *ab initio* calculation with the jellium-based one. Using this pseudopotential as a correction to the standard jellium model, one can introduce effects of the sp²-hybridization of carbon atomic orbitals into the jellium model and relate parameters of the model with the features of the system obtained from the more precise calculation. By means of the presented pseudopotential, a relatively simple jellium model acquires more physical sense

and parameters of the model obtain a clear physical justification. Hereby, we confirm the relevance of using the jellium model for the description of fullerenes. Investigating two molecules, C_{60} and C_{20} , we show that the results obtained have a common origin and that they could be also extended to other highly symmetric fullerenes.

The atomic system of units, $m_e = |e| = \hbar = 1$, is used throughout the paper.

2. Methods of investigation

2.1. Jellium model

In this paper, the fullerenes C_{60} and C_{20} are treated within the jellium model which is based on an assumption that a many-electron system is considered as a sum of two interacting subsystems: a valence electrons subsystem and a positively charged ionic core. One of the stable isomers of C_{20} corresponds geometrically to the regular dodecahedron [23] and, like the truncated icosahedron C_{60} , has the symmetry of the I_h point group which is very close to spherical symmetry. Therefore, a detailed ionic structure of the systems under study is substituted by the uniform spherically symmetric distribution of the positive charge, in the field of which the motion of the valence electrons is considered [9].

The valence $2s^2 2p^2$ electrons in each carbon atom form a cloud of delocalized electrons, while the inner-shell $1s^2$ electrons are treated as frozen and not taken into consideration. Thereby, we consider 240 delocalized electrons in C_{60} and 80 electrons in C_{20} . The valence electrons are moving in a spherically symmetric central field, so one can construct the electronic configuration described by the unique set of quantum numbers $\{n, l\}$ where n and l are the principal and orbital quantum numbers, respectively.

Since it is commonly acknowledged [24–26] that C_{60} , as well as other fullerenes, is formed from fragments of planar graphite sheets, it is natural to match the σ - and π -orbitals of graphite to the nodeless and the single-node wavefunctions of a fullerene, respectively [27]. Carbon atoms within a graphite sheet are connected by σ -bonds, whereas different sheets are connected by π -bonds. In the fullerene, the nodeless σ -orbitals are localized at the radius of the ionic core while the single-node π -orbitals are oriented perpendicularly to the fullerene surface. The ratio of σ - to π -orbitals in C_{60} should be equal to 3 : 1 due to the sp^2 -hybridization of carbon orbitals [28]. Thereby, the electronic configuration of the delocalized electrons in C_{60} is written in the form [13]:

$$1s^2 2p^6 3d^{10} 4f^{14} 5g^{18} 6h^{22} 7i^{26} 8k^{30} 9l^{34} 10m^{18} \\ 2s^2 3p^6 4d^{10} 5f^{14} 6g^{18} 7h^{10}.$$

Radial wavefunctions of the $1s \dots 10m$ shells are nodeless, while the wavefunctions of the $2s \dots 7h$ shells have one radial node each.

Using the same methodology, one defines the electronic configuration of the 80 delocalized electrons in C_{20} as follows:

$$1s^2 2p^6 3d^{10} 4f^{14} 5g^{18} 6h^{10} 2s^2 3p^6 4d^{10} 5f^2.$$

Within the jellium model the fullerene core of the charged carbon ions, C^{4+} , is described as a positively charged spherical layer of a finite thickness $\Delta R = R_2 - R_1$. The thickness ΔR is chosen to be equal to 1.5 Å which corresponds to a typical diameter of a carbon atom [29] and refers to experimental data from [18]. The potential of the core may be written as:

$$U_{\text{core}}(r) = -N \times \begin{cases} \frac{3R_2^2 - R_1^2}{2R_2^3 - R_1^3}, & r < R_1 \\ \frac{1}{2(R_2^3 - R_1^3)} \left(3R_2^2 - r^2 \left(1 + \frac{2R_1^3}{r^3} \right) \right), & R_1 \leq r \leq R_2 \\ \frac{1}{r}, & r > R_2 \end{cases}, \quad (1)$$

where N is the number of delocalized electrons in a fullerene ($N = 240$ in C_{60} and $N = 80$ in C_{20}), $R_1 = R - \Delta R/2$ and $R_2 = R + \Delta R/2$ with R standing for a fullerene radius ($R_{C_{60}} = 3.54$ Å and $R_{C_{20}} = 2.04$ Å [30]).

The electronic subsystem is treated within the local density approximation (LDA). Single-electron wave functions $\phi_{nlm}(\mathbf{r})$ and the corresponding energies ε_{nl} are determined from a system of self-consistent Kohn-Sham equations:

$$\left[-\frac{\Delta}{2} + U_{\text{eff}}(\mathbf{r}) \right] \phi_{nlm}(\mathbf{r}) = \varepsilon_{nl} \phi_{nlm}(\mathbf{r}), \quad (2)$$

$$U_{\text{eff}}(\mathbf{r}) = U_{\text{core}}(r) + \int \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}' + U_{\text{XC}}^{\text{LDA}}(\mathbf{r}), \quad (3)$$

$$\rho(\mathbf{r}) = \sum_{nl} \sum_{m=-l}^l \frac{N_{nl}}{2(2l+1)} |\phi_{nlm}(\mathbf{r})|^2, \quad (4)$$

where N_{nl} is a number of electrons in the nl -shell. The exchange-correlation potential $U_{\text{XC}}^{\text{LDA}}(\mathbf{r})$ is represented as a sum of the Slater exchange potential and a correlation potential:

$$U_{\text{XC}}^{\text{LDA}}(\mathbf{r}) = U_{\text{X}}(\mathbf{r}) + U_{\text{C}}(\mathbf{r}) = -\left(\frac{3}{\pi}\right)^{1/3} \rho^{1/3}(\mathbf{r}) + U_{\text{C}}(\mathbf{r}). \quad (5)$$

In the calculations, we used Perdew and Zunger parameterization of the correlation potential [31] which is presented in the form

$$U_{\text{C}}(r_s) = \varepsilon_{\text{C}}(r_s) \frac{1 + 1.229\sqrt{r_s} + 0.444r_s}{1 + 1.053\sqrt{r_s} + 0.333r_s}, \quad (6)$$

$$\varepsilon_{\text{C}}(r_s) = -\frac{0.142}{1 + 1.053\sqrt{r_s} + 0.333r_s}, \quad (7)$$

where $r_s(\mathbf{r}) = (4\pi\rho(\mathbf{r})/3)^{-1/3}$ is the local Wigner-Seitz radius for the electronic subsystem and $\varepsilon_{\text{C}}(r_s)$ is the correlation energy per electron.

2.2. *Ab initio* calculations

The *ab initio* calculations were performed using the Gaussian 09 package [5]. For the description of the C₆₀ and C₂₀ fullerenes we used the split-valence triple-zeta basis set 6-311+G(d) with an additional set of polarization and diffuse functions. The systems were calculated by means of the density functional theory. To account for the exchange and correlation corrections, the Slater exchange functional [32] and the local Perdew functional (the so-called Perdew Local, PL) [31] were used. By applying these rather simple functionals we wanted to achieve a full similarity in the description of the electronic subsystem within the jellium model and the *ab initio* approaches.

The total electrostatic potential of the system is represented as a sum of the nuclear and electronic parts:

$$U_{\text{tot}}(\mathbf{r}) = U_{\text{n}}(\mathbf{r}) + U_{\text{el}}(\mathbf{r}) = - \sum_A \frac{Z_A}{|\mathbf{r} - \mathbf{R}_A|} + \int \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}' . \quad (8)$$

The electron density $\rho(\mathbf{r})$ and the potential $U_{\text{n}}(\mathbf{r})$ created by all carbon ions, C⁴⁺(1s²), were extracted from the Gaussian output file with the help of the Multiwfn software [33]. The potential $U_{\text{el}}(\mathbf{r})$ created by the delocalized electrons was calculated separately using the extracted electron density.

The jellium model treats the fullerenes C₆₀ and C₂₀ as spherically symmetric objects while a more precise *ab initio* calculation accounts for the real icosahedral symmetry of the molecules. Therefore, to draw an analogy between the two methods we averaged the exact electrostatic potential and the electron density over the directions of the position vector \mathbf{r} :

$$\begin{aligned} \bar{U}_{\text{tot}}(r) &= \bar{U}_{\text{n}}(r) + \bar{U}_{\text{el}}(r) , \\ \bar{U}_{\text{i}}(r) &= \frac{1}{4\pi} \int U_{\text{i}}(\mathbf{r}) d\Omega \quad (\text{i} = \text{tot}, \text{n}, \text{el}) , \\ \bar{\rho}(r) &= \frac{1}{4\pi} \int \rho(\mathbf{r}) d\Omega . \end{aligned} \quad (9)$$

The averaged electron density includes only delocalized electrons, while the inner electron orbitals are excluded from the consideration.

3. Numerical results

In this section, we compare the results of the *ab initio* and the jellium model calculations for C₆₀ and C₂₀. The fullerene C₆₀ is discussed in detail below. The results for the C₂₀ molecule and the comparison with C₆₀ are discussed further in this section.

Using the methodology implemented in a number of papers [12, 16, 18, 21], we add a negative SW pseudopotential U_{SW} to the core potential (1):

$$U_{\text{core}}(r) \rightarrow \begin{cases} U_{\text{core}}(r) + U_{\text{SW}} & , R_1 \leq r \leq R_2 \\ U_{\text{core}}(r) & , \text{otherwise} \end{cases} . \quad (10)$$

The depth of the SW potential was chosen to obtain the same value of the outer-shell ionization potential as the defined one from the quantum-chemical calculation. The pseudopotential U_{SW} is shown by the dashed red curve in the lower panel of figure 3.

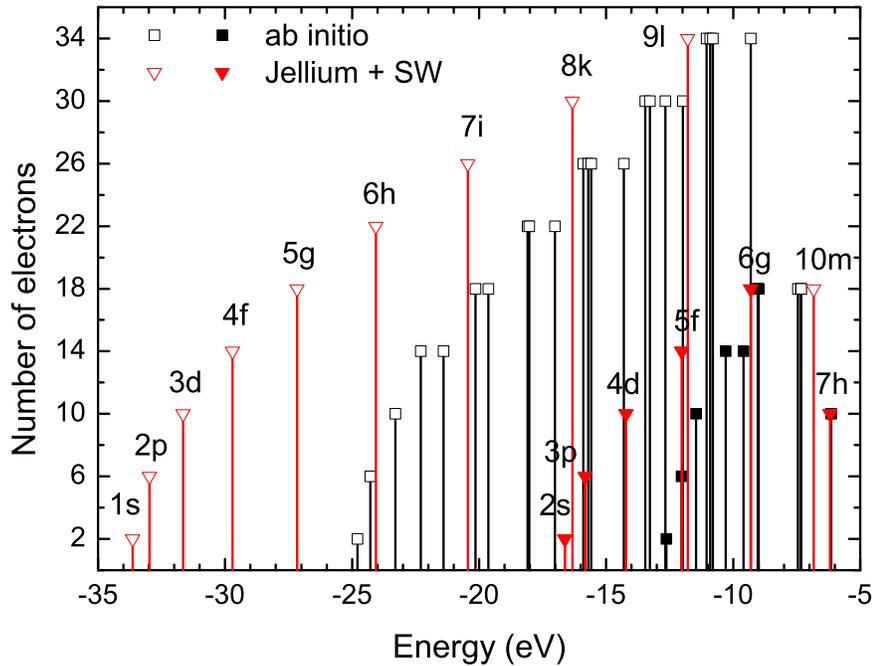


Figure 1. Single-electron energy levels of C_{60} obtained from the *ab initio* calculation (empty and filled squares) and within the jellium model with an additional square-well (SW) pseudopotential (empty and filled triangles). Nodeless σ -orbitals and single-node π -orbitals are labeled by empty and filled symbols, respectively.

Single-electron energy spectra obtained from the *ab initio* calculation and within the jellium model are presented in figure 1. For the ease of perception, the height of levels of split states (black lines) corresponds to the occupation of shells within the jellium model (red lines). Ionization potentials of several outer shells (6g, 10m and 7h) are in a good agreement with the *ab initio* results while the remainder of the jellium spectrum is significantly broadened and differs from the more precise calculation. It should be mentioned that none of the various jellium-based calculations of C_{60} performed earlier [12,13,16,17,20,21] can produce the quantitative agreement of the single-electron spectrum with that one obtained from the more precise *ab initio* calculation.

The radial density of the delocalized electrons obtained within the two approaches is presented in figure 2. It is shown that the standard jellium model without any corrections (dashed red curve) fails to represent the results of the *ab initio* calculation (black curve). The additional SW pseudopotential does not modify the density distribution significantly (solid red curve).

As shown in figures 1 and 2, the jellium model with a simple additional

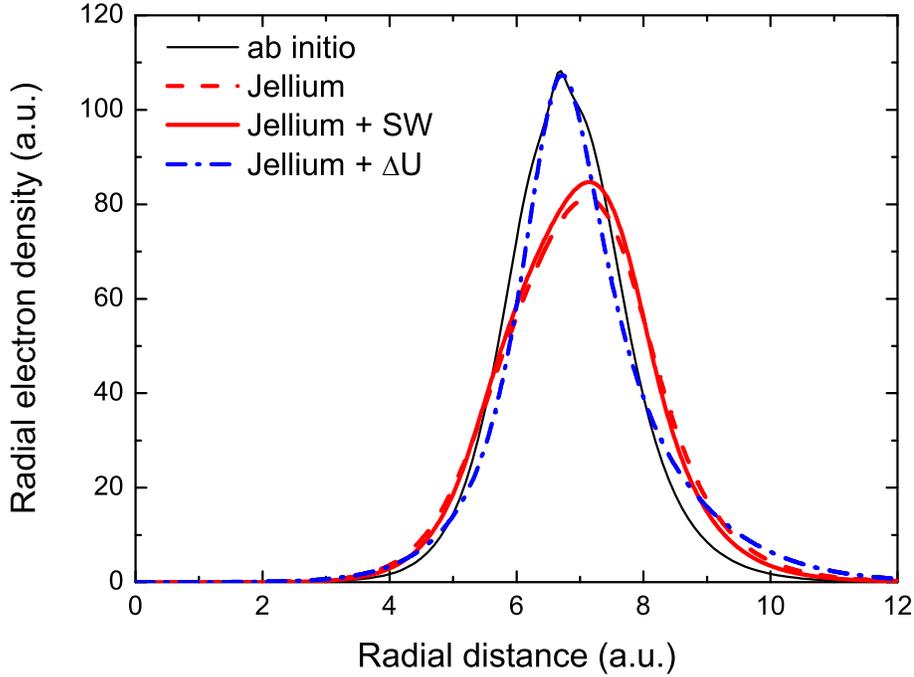


Figure 2. Radial electron density of C_{60} obtained from the *ab initio* calculation (solid black curve) and calculated by means of the jellium model: the standard one (dashed red curve), with the additional SW pseudopotential (solid red curve) and with the additional pseudopotential ΔU (dash-dotted blue curve).

pseudopotential represents neither the single-electron energy spectrum nor the electron density distribution. As opposed to more precise quantum chemistry methods, the jellium model does not take into account chemical features of the fullerene, such as hybridization of atomic orbitals in the formation of chemical bonding. However, the jellium model can be improved by means of a more sophisticated pseudopotential which will allow one to describe chemical properties of the real system. In this paper, we introduce the correction as a difference between the total electrostatic potential of the system obtained from the *ab initio* calculation and the one obtained within the jellium model:

$$\Delta U(r) = U_{\text{tot}}^{\text{QC}}(r) - U_{\text{tot}}^{\text{jel}}(r) , \quad (11)$$

where $U_{\text{tot}}^{\text{QC}}(r)$ is defined by Eq. (8), and the potential $U_{\text{tot}}^{\text{jel}}(r)$ obtained within the jellium model is defined as:

$$U_{\text{tot}}^{\text{jel}}(r) = U_{\text{core}}(r) + \int \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}' . \quad (12)$$

The total potentials $U_{\text{tot}}^{\text{QC}}(r)$ and $U_{\text{tot}}^{\text{jel}}(r)$ of C_{60} as well as their difference $\Delta U(r)$ are shown in figure 3.

We note that previously several spiritually close averaged pseudopotentials have been introduced to correct the jellium model. For instance, it was done in the case of inhomogeneous electron gas on metal surfaces [34, 35] and for spherically symmetric metallic clusters [36, 37].

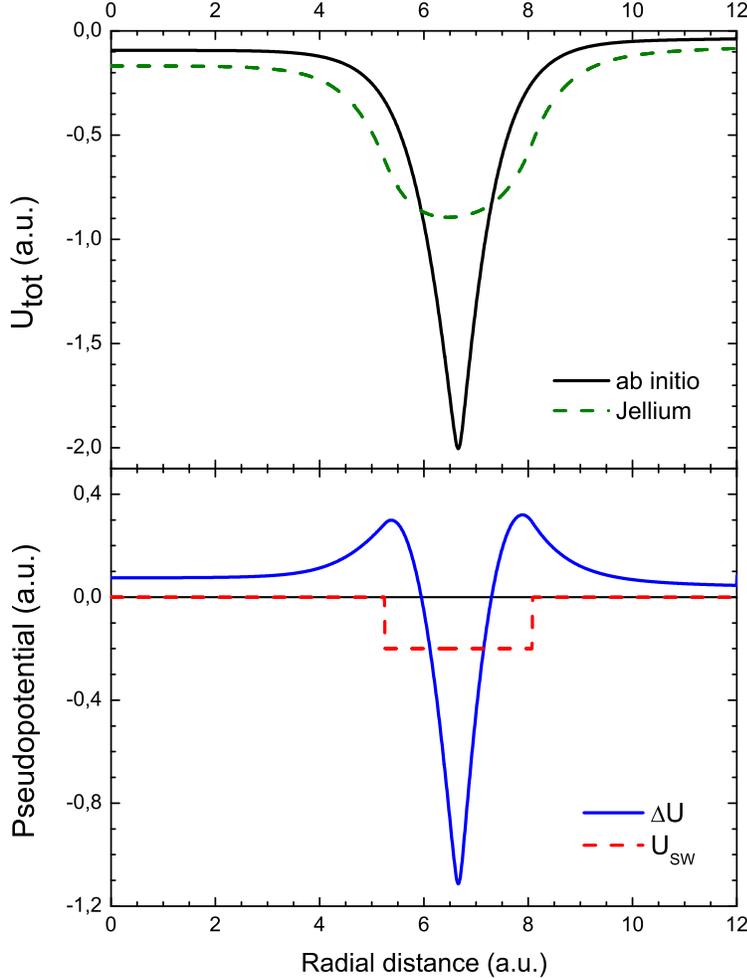


Figure 3. Upper panel: total electrostatic potential of C_{60} obtained from the *ab initio* quantum chemistry calculation (solid curve) and within the jellium model (dashed curve). Lower panel: the difference ΔU between the total electrostatic potential of C_{60} calculated by the *ab initio* methods and the one calculated within the jellium model (solid blue curve). The SW pseudopotential U_{SW} is also shown for the comparison (dashed red curve).

As opposed to the SW pseudopotential which affects equally all electrons of the system, ΔU is an alternating-sign pseudopotential (see the lower panel of figure 3), therefore it is attractive in the vicinity of the fullerene ionic core and repulsive at larger distances from the fullerene surface. This means that such a potential affects differently the σ - and π -electrons of C_{60} which are located on the surface of the molecule and perpendicularly to it, respectively. Therefore, one can conclude that by means of a such

potential it is possible to account, to some extent, for the hybridization properties of the fullerene.

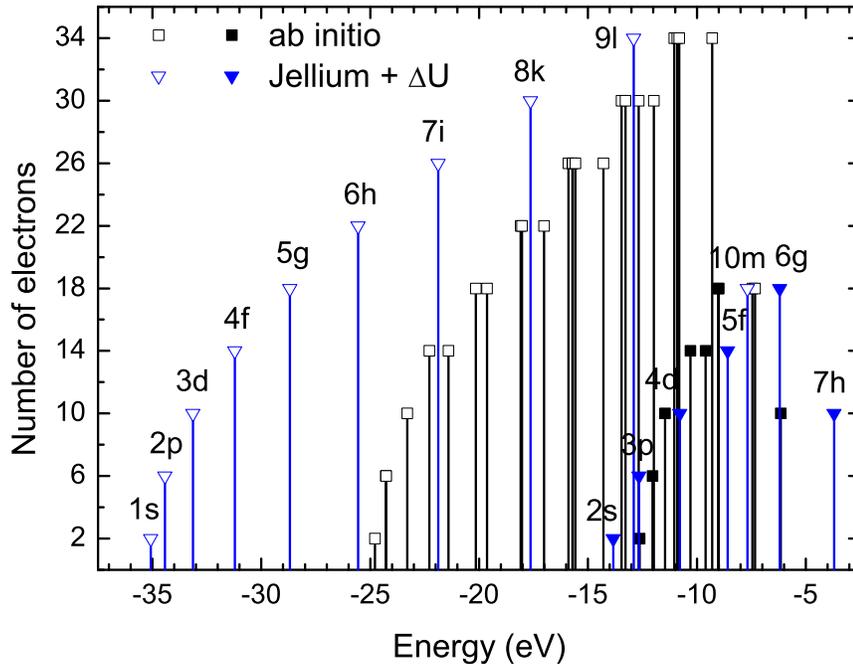


Figure 4. Single-electron energy levels of C_{60} obtained from the *ab initio* calculation (empty and filled squares) and within the modified jellium model with an additional pseudopotential ΔU (empty and filled triangles). Nodeless σ -orbitals and single-node π -orbitals are labeled by empty and filled symbols, respectively.

The single-electron energy spectrum obtained within the "modified" jellium model with ΔU taken as an additional pseudopotential is presented in figure 4. The modification allows one to obtain a better agreement of the jellium calculation with the *ab initio* one for the inner single-node $2s \dots 5f$ orbitals. On the contrary, it shifts the $6g$ and $7h$ ionization potentials by 2.8 and 2.5 eV, respectively, and still does not lead to a better quantitative agreement for the whole spectrum (see figure 4).

Introduction of the alternating-sign pseudopotential ΔU allows one to improve significantly the electron density distribution (see the dash-dotted blue curve in figure 2). The difference between the *ab initio* calculated electron density and the one from the jellium model calculation in the spatial region $8 - 12$ a.u. may contribute to the shift of $6g$ and $7h$ ionization potentials (see figure 4).

Below we present and discuss the results for the C_{20} molecule. Following the formalism described above for C_{60} , the additional pseudopotential ΔU is introduced as a difference between the total electrostatic potential of C_{20} obtained from the *ab initio* quantum-chemical calculation and the one obtained within the jellium model. Figure 5 represents the correction ΔU calculated for C_{60} and C_{20} . It is shown that ΔU

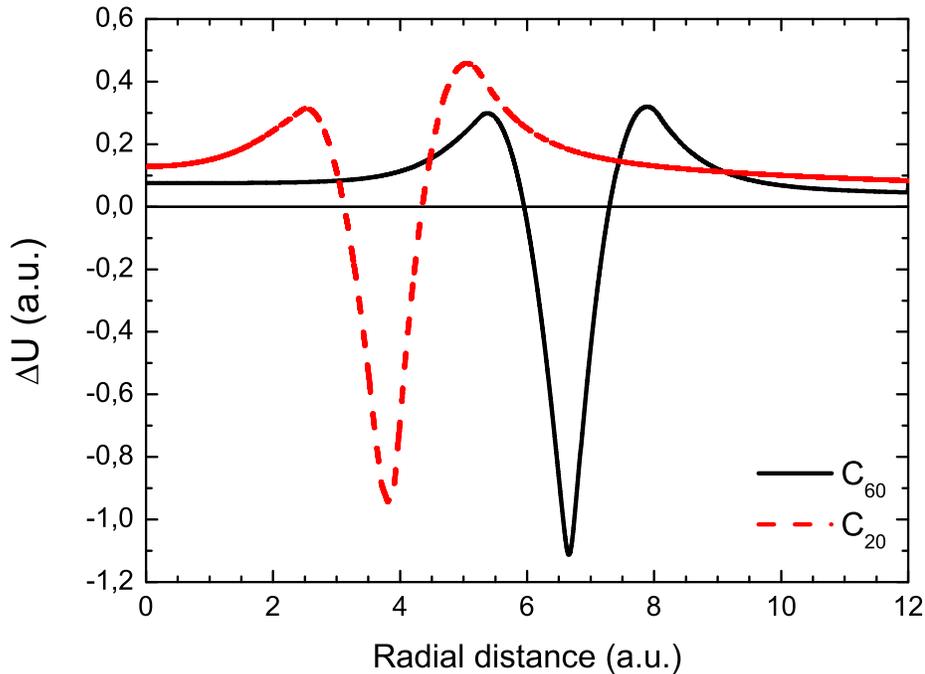


Figure 5. The additional pseudopotential ΔU in cases of C_{60} (solid curve) and C_{20} (dashed curve).

has a similar alternating-sign shape for both molecules but it is more asymmetric in the case of C_{20} .

The single-electron energy spectra of C_{20} are presented in figure 6. The pseudopotential ΔU does not influence significantly on all nodeless orbitals while the single-node orbitals are shifted. This shift leads to a better agreement of the *ab initio* and jellium calculations for 2s and 3p shells but gives a wrong value for the outer 4d and 5f ionization potentials.

The additional pseudopotential ΔU exerts a similar influence on the electron density distribution of C_{20} , as in case of C_{60} (see figure 7). In comparison with a standard jellium model (dashed red curve), the modified one improves the density distribution in the vicinity of the fullerene core (dash-dotted blue curve) but the electron density is spread partly to the spatial region 5 – 9 a.u.

Having considered two different fullerenes within the spherical jellium model, one can conclude that the precise description of single-electron energy spectra of these systems by means of the jellium model is very difficult and elusive task, though such an approach produces mostly the right sequence of energy levels. Additional pseudopotentials allow one to obtain the right value of the ionization potential only for several outer shells but do not alter the overall situation significantly. At the same time, we suppose that by improving the ground-state density distribution with the introduced

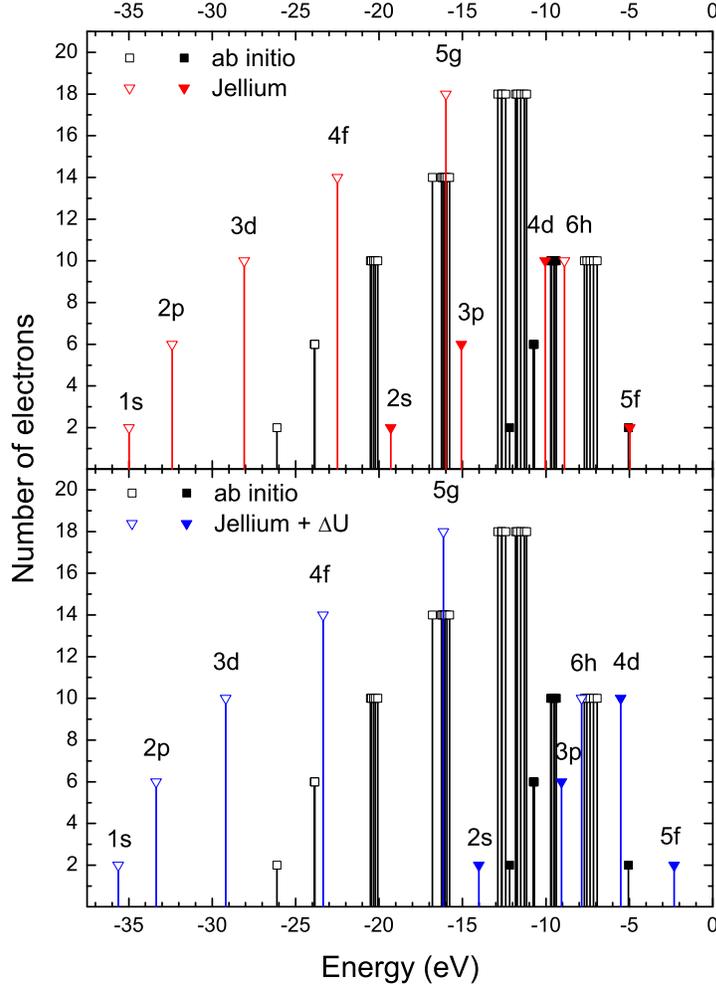


Figure 6. Single-electron energy levels of C_{20} obtained from the *ab initio* calculation (empty and filled squares) and within the jellium model (empty and filled triangles): the standard one (upper panel) and the modified one (lower panel). Nodeless σ -orbitals and single-node π -orbitals are labeled by empty and filled symbols, respectively.

pseudopotential one can achieve higher accuracy while constructing the photoionization amplitudes.

The obtained pseudopotentials for C_{60} and C_{20} can be well fitted by three Lorentz functions. The result of the fitting procedure is presented in figure 8. Supposing $\Delta U(r) \equiv y(x)$, the resulting fitting function could be defined in the following form:

$$y(x) = y_0 + \sum_{i=1}^3 \frac{2A_i}{\pi} \frac{w_i}{4(x - x_{c_i})^2 + w_i^2}, \quad (13)$$

where y_0 is the offset constant, x_c is the position of the peak maximum, w is the full-width at half-maximum and A is the normalization factor. The obtained values of these parameters are presented in table 1.

As was shown above, the pseudopotential ΔU has a more asymmetric form in the

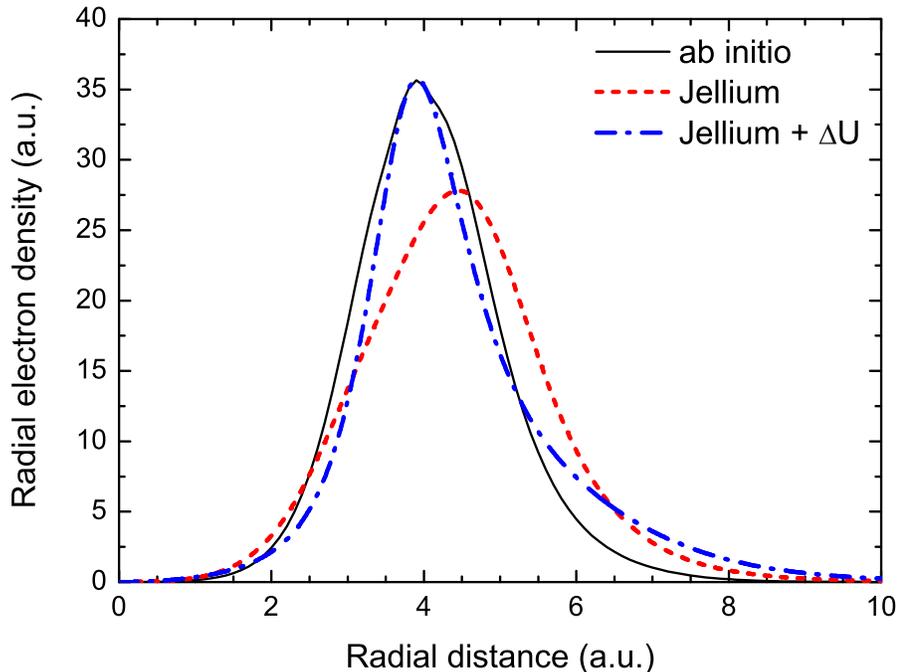


Figure 7. Radial electron density of C_{20} obtained from the *ab initio* calculation (solid curve) and calculated within the jellium model, the standard one (dashed curve) and with the additional pseudopotential ΔU (dash-dotted curve).

Table 1. Parameters of the Lorentz functions used for the fitting the pseudopotential ΔU for C_{60} and C_{20} .

	y_0	x_{c_1}	w_1	A_1	x_{c_2}	w_2	A_2	x_{c_3}	w_3	A_3
C_{60}	0.064	5.453	1.425	0.727	6.647	0.785	-1.610	7.763	1.264	0.727
C_{20}	0.092	2.650	1.719	0.815	3.797	0.939	-2.053	4.779	1.934	1.606

case of C_{20} than in the case of C_{60} ; therefore, it should affect differently the π -electrons of these systems. Figure 9 represents the radial density of π -electrons in the C_{60} and C_{20} molecules obtained within the standard jellium model as well as the one augmented by ΔU . The minimum of the π -electron density distribution is located at 6.78 a.u. for C_{60} and 4.03 a.u. for C_{20} . These values are slightly shifted from the mean radius of the molecules, which equals 6.67 a.u. and 3.86 a.u., respectively. It is shown that due to the hybridization-related correction ΔU , π -electrons in both systems are distributed non-uniformly in the inner and outer regions of the molecules.

To estimate a relative degree of spill-out of the π -electrons to the outer region of the fullerene molecules, we normalized the density distributions by dividing them by the number of the π -electrons in each system. We also shifted the π -electron density of C_{60} to the one of C_{20} to match the minima of the curves. The result is presented in figure

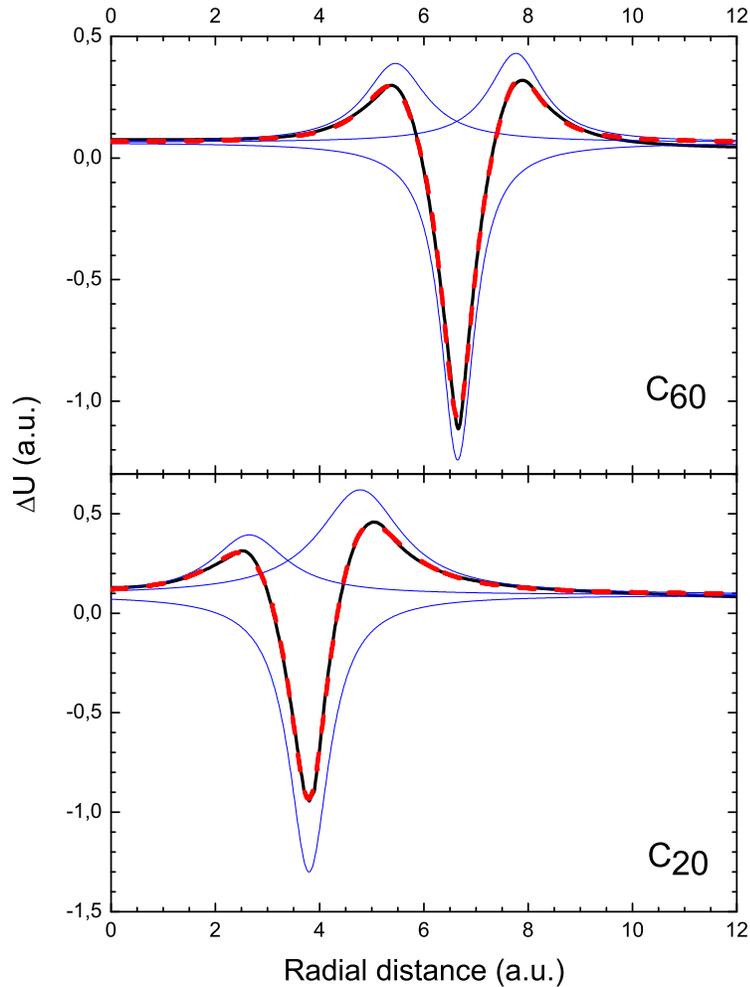


Figure 8. Pseudopotential ΔU for the C_{60} (upper panel) and C_{20} (lower panel) molecules. The initial curve is presented by the thick solid (black) line, dashed (red) line represents the fitting curve constructed as a sum of three primitive Lorentz functions (thin blue lines).

10. It is shown that the profile of the π -electron density in C_{60} differs from the one in C_{20} . Due to the smaller radius of the molecule and a bigger curvature of the fullerene surface, π -electrons in C_{20} are spilled out further than in the case of C_{60} . On the basis of this comparison, we suppose that for larger fullerenes, such as C_{240} , π -electrons should be distributed more uniformly due to a smaller curvature of the surface of the molecule.

4. Conclusion

To conclude, we have introduced a new type of correction for description of the fullerenes C_{60} and C_{20} within the spherically symmetric jellium model. The correction is represented as an additional pseudopotential which originates from the difference between the precise *ab initio* calculation and the one within the jellium model. Due to

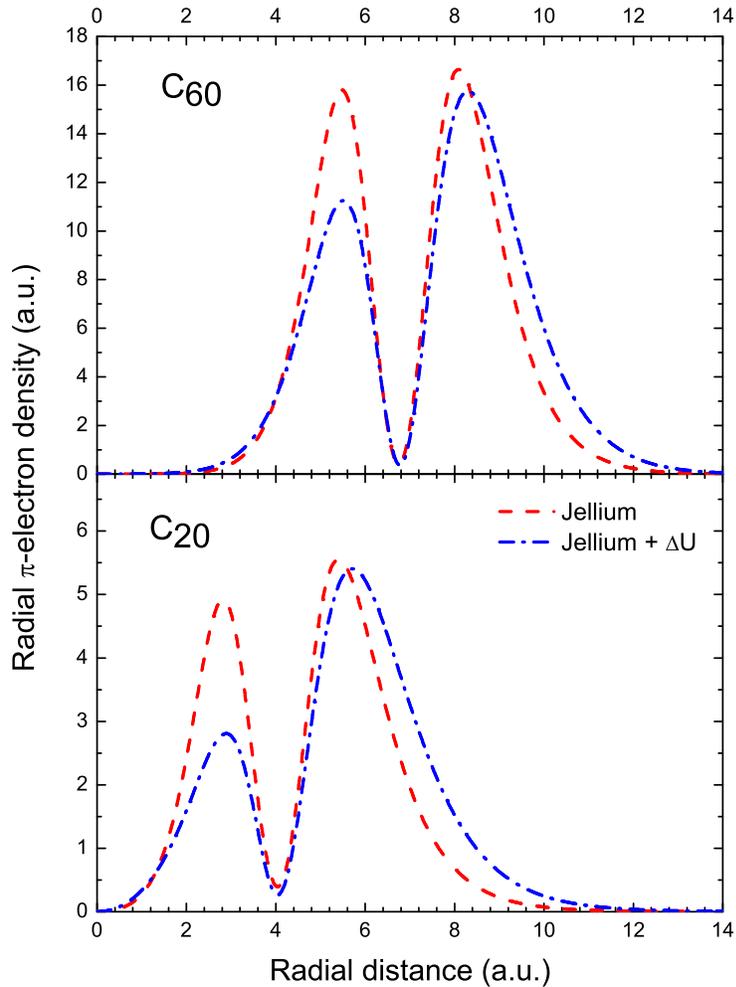


Figure 9. Radial density of π -electrons in C_{60} (upper panel) and C_{20} (lower panel) calculated within the standard jellium model (dashed red curve) and the modified jellium model with the presence of ΔU (dash-dotted blue curve).

the alternating-sign shape of the potential, it affects the σ - and π -electrons of the system differently. Therefore, this potential allows one to mimic partially the sp^2 -hybridization, which occurs in formation of fullerenes, and, thus, to import the hybridization effects into the standard jellium model. We have shown that the correction used improves significantly the electron density distribution as compared to the standard jellium model and the one with an additional square-well pseudopotential. Like the other previously used corrections, it does not allow one to obtain a quantitative agreement with an *ab initio* calculation for the single-electron energy spectrum but reproduces the sequence of energy levels corresponding to the one following from the more precise quantum-chemical calculation.

As the next step of this work, the correction to the jellium model, introduced in this paper, will be utilized further for the calculation of the dynamic response of fullerenes in

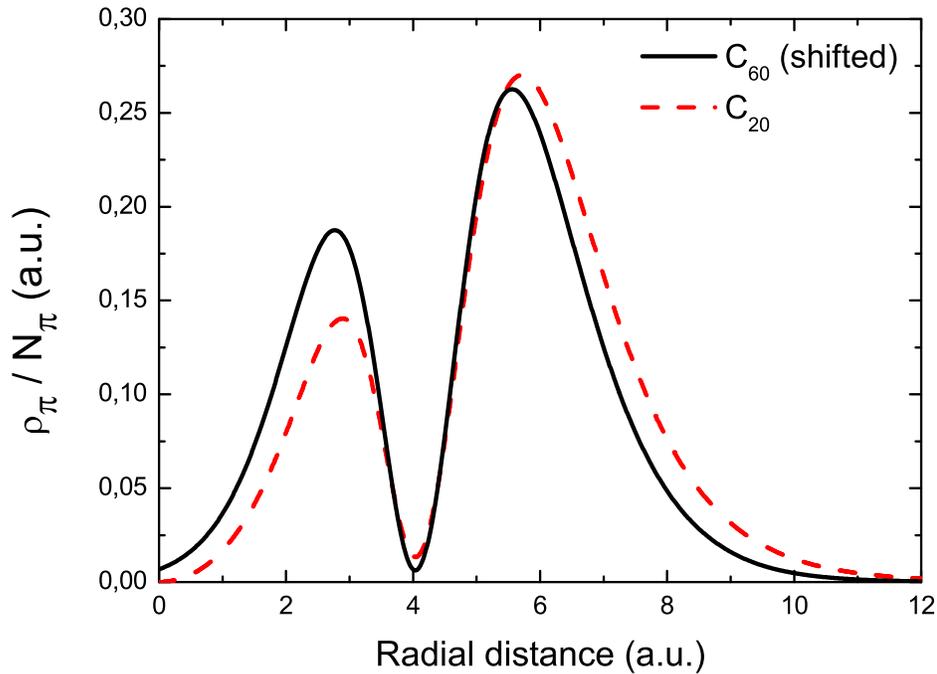


Figure 10. Radial π -electron densities, ρ_π , of the C_{60} and C_{20} fullerenes normalized by the number of the π -electrons, N_π , in each system. The density distribution of C_{60} is shifted to match the minima of the two curves (see the text for more explanation).

the processes of photon and electron impact excitation. We suppose that improving the ground-state density distribution with the introduced pseudopotential it is possible to get an accurate description of the excitation processes of fullerenes. Particular attention will be paid on the study of collective electron excitations. This work is currently in progress and the results will be presented elsewhere. An implementation of the presented formalism for larger fullerene molecules, nanotubes etc. could be another topic of further investigations.

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