Electron elastic scattering off polarizable $A@C_{60}$: The complete study within a particular theory

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A deeper insight into electron elastic scattering off endohedral fullerenes $A@C_{60}$ is provided. The study accounts for polarization of both the encapsulated atom $A$ and $C_{60}$ cage by an incident electron. It is carried out in the framework of the combination of both a model and the first-principle approximations. A core principle of the model is that the $C_{60}$ cage itself is presented by an attractive spherical potential of a certain inner radius, thickness, and depth. The main idea of the first-principle approximation is that the polarization of $A@C_{60}$ by an incident electron is accounted with the help of the Dyson equation for the self-energy part of the Green’s function of an incident electron. Calculations are performed for, and comparison is made between the individual cases: (a) when $A@C_{60}$ is regarded as a static system, (b) when $C_{60}$ is a static cage, but the encapsulated atom is polarizable, (c) when both $C_{60}$ and $A$ are polarized simultaneously but independently of each other, and (d), as the most general scenario, when polarizabilities of $C_{60}$ and $A$ are coupled. Spectacular similarities and discrepancies between results of each of the exploited approximations are demonstrated. Revealed features of the overall significant impact of $A@C_{60}$ polarization by an incident electron on its elastic scattering off $A@C_{60}$ are demonstrated. Choosing Ne, Xe, and Ba as “probing” atoms, the dependence of $e + A@C_{60}$ scattering on the size and polarizability of the encapsulated atom is unraveled.

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I. INTRODUCTION

Electron elastic scattering off quantum targets is an important fundamental phenomenon of nature. It has significance to both the basic and applied sciences and technologies. To date, however, the knowledge on electron elastic scattering by such quantum targets as endohedral fullerenes $A@C_{60}$, where an atom $A$ is encapsulated inside the hollow interior of a $C_{60}$ molecule, is rudimentary. This is not accidental, since the comprehensive description of electron scattering, especially of a low-energy electron scattering, by a multielectron target is too challenging for theorists even with regard to a free atom, not to mention a complicated and more multifaceted $A@C_{60}$ target. It is, perhaps, for this reason that so far there have been only a few attempts undertaken by theorists \cite{1, 2} to advance into the world of low-energy electron scattering off $A@C_{60}$. Specifically, to address the problem, a model static Hartree-Fock (HF) approximation was employed in Refs. \cite{1, 2}. Additionally, in Ref. \cite{3}, a provisional attempt was made to evaluate the impact of polarization of $C_{60}$ on $e + A@C_{60}$ scattering. Despite a number of interesting features of electron scattering off $A@C_{60}$ were predicted, the drawback of those studies was obvious. A further attempt to get a better understanding of $e + A@C_{60}$ scattering was later undertaken in Ref. \cite{4}. There, the model $C_{60}$ cage was kept static (“frozen”), but the encapsulated atom $A$ was “unfrozen”, i.e., regarded as a polarizable atom. A significant impact of its dynamical polarization (in the presence of static $C_{60}$) by an incident electron on $e + A@C_{60}$ scattering was revealed.

That was achieved by exploiting the Dyson formalism \cite{4, 5, 6} for the self-energy part of the Green’s function of a scattered electron. A remained drawback of work \cite{4} was the neglect of polarization of $C_{60}$ cage itself by incident electrons. It remained unclear how to overcome this drawback in an efficient and yet physically transparent way. Recently, an idea of how to address the problem of electron scattering off a fully polarizable $A@C_{60}$ in a reasonably simple approximation was put forward in Ref. \cite{5}.

The same idea as in Ref. \cite{5} is exploited in the present work as well, in order to get a better insight into $e + A@C_{60}$ scattering by accounting for polarization of both $C_{60}$ and $A$. The emphasis is not only on the study of the significance of the polarization effect in $e + A@C_{60}$ scattering, but on the sensitivity of the scattering process to both the size and polarizability of the encapsulated atom $A$. We choose Ne, Xe, and Ba as test-atoms and explore electron elastic scattering off such $A@C_{60}$ systems in the region of about a zero to a few eV of the electron energy, where the most interesting effects occur.

Atomic units (a.u.) are used throughout the text unless specified otherwise.

II. THEORETICAL CONCEPTS

To give the reader a heads-up on how the problem of $e + A@C_{60}$ scattering is going to be addressed in the present work, before indulging into details, the key points to mention are as follows. As the first step, the $C_{60}$
cage is approximated by an attractive square-well (in
the radial coordinate \( r \)) static potential \( U_c(r) \) of cer-
tain depth \( U_0 \), inner radius \( r_0 \), and thickness \( \Delta \). As a
second step, in order to account for the effect of polari-
zation of \( C_{60} \) by an incident electron, the \( C_{60} \) cage is
modeled by a modified potential \( V_{C_{60}}(r) = U_c(r) + V_r(r) \).
Here, \( V_r(r) \) is the long-range static polarization poten-
tial of \( C_{60} \): \( V_r(r) = -\alpha/\left[2\left(r^2 + b^2\right)^{3/2}\right] \),
where \( \alpha \) is the static polarizability of \( C_{60} \) and \( b \) is a parameter of
the order of \( r_0 \). Next, the wavefunctions of incident elec-
trons and electrons of the encapsulated atom \( A \) are cal-
culated in the potential \( V_{A@C_{60}}(r) \) which is the sum of
\( V_{C_{60}}(r) \) and the atomic Hartree-Fock potential \( V_A^{HF}(r) \):
\( V_{A@C_{60}}(r) = V_{C_{60}}(r) + V_A^{HF}(r) \). The thus found func-
tions are substituted into the Dyson’s equation for self-
energy part of the one-electron Green function \( \Sigma \) of an
incident electron. In the present work, \( \Sigma \) is defined such
that it accounts for excitations of both atomic electrons
and electrons of the \( C_{60} \) cage in the presence of polar-
ized \( C_{60} \). Then, the Dyson equation for \( \Sigma \) is solved with
a reasonable assumption that \( r_p \gg r_0 \gg r_A \). Here,
\( r_p \) is the electron-projectile distance from the enter
of \( C_{60} \) and \( r_A \) is the radius of the encapsulated atom \( A \).
With the thus determined \( \Sigma \), electron elastic-scattering
phase shifts upon electron collision with a fully polariz-
able \( A@C_{60} \) are found and, eventually, the electron scat-
tering cross sections are calculated, as the last step of the
study.

A. Model static HF approximation: “frozen” \( A@C_{60} \)

In the present work, as in Refs. \[1, 2\], the \( C_{60} \) cage is
modeled by an attractive spherical potential \( U_c(r) \):

\[
U_c(r) = \begin{cases} 
-U_0, & \text{if } r_0 \leq r \leq r_0 + \Delta \\
0, & \text{otherwise}
\end{cases}
\]

(1)

Here, \( r_0 \), \( \Delta \), and \( U_0 \) are the inner radius, thickness, and
depth of the potential well, respectively.

The wavefunctions \( \psi_{n\ell m_i}(r, \sigma) = r^{-1} P_{\ell}(r) Y_{l\sigma}(\theta, \phi) \chi_{m_i}(\sigma) \) and binding energies \( \epsilon_{nl} \)
of atomic electrons are the solutions of a system of the “endo-
hedral” HF equations:

\[
\frac{\Delta}{2} - \frac{Z}{r} + U_c(r) \psi_i(x) + \sum_{j=1}^{Z} \int \frac{\psi_j^*(x')}{|x - x'|} \times \left[ \psi_j(x') \psi_i(x) - \psi_i(x') \psi_j(x) \right] dx' = \epsilon \psi_i(x).
\]

(2)

Here, \( n \), \( \ell \), \( m_i \) and \( m_s \) is the standard set of quantum
numbers of an electron in a central field, \( \sigma \) is the elec-
tron spin variable, \( Z \) is the nuclear charge of the atom,
\( x \equiv (r, \sigma) \), and the integration over \( x \) implies both the
integration over \( r \) and summation over \( \sigma \). Eq. (2) differs
from the ordinary HF equation for a free atom by the presence of
the \( U_c(r) \) potential in there. This equation is first solved in order to calculate the electronic
ground-state wavefunctions of the encapsulated atom. Once the electronic ground-state wavefunctions are
determined, they are plugged back into Eq. (2) in place of \( \psi_j(x') \) and \( \psi_j(x) \) in order to calculate the electronic
wavefunctions of scattering-states \( \psi_i(x) \) and their radial parts \( P_{\ell\ell}(r) \equiv \Psi_{\ell\ell}(r) \) in Eq. (2).

Corresponding electron elastic-scattering phase shifts \( \delta_{\ell}(k) \) are then determined by referring to \( P_{\ell\ell}(r) \) at large
\( r \):

\[
P_{\ell\ell}(r) \rightarrow \sqrt{\frac{2}{\pi}} \sin \left( k r - \frac{\pi \ell}{2} + \delta_{\ell}(k) \right).
\]

(3)

Here, \( P_{\ell\ell}(r) \) is normalized to \( \delta(k - k') \), where \( k \) and \( k' \)
are the wavenumbers of the incident and scattered elec-
trons, respectively. The total electron elastic-scattering
cross section \( \sigma_{el}(\varepsilon) \) is then found in accordance with the
well-known formula for electron scattering by a central-
potential field:

\[
\sigma_{el}(\varepsilon) = \frac{4\pi}{k^2} \sum_{\ell=0}^{\infty} (2\ell + 1) \sin^2 \delta_{\ell}(k).
\]

(4)

This approach solves the problem of \( e + A@C_{60} \) scatter-
ing in a static approximation, i.e., without account for
polarization of the \( A@C_{60} \) system by incident electrons.

In the literature, some inconsistency is present in
choosing the magnitudes of \( \Delta \), \( U_0 \) and \( r_0 \) of the model
potential \( U_c(r) \) for \( C_{60} \), for example: \( r_0 = 5.8 \), \( \Delta = 1.9 \)
and \( U_0 = 0.302 \) a.u. \[11\] (and references therein), or
\( r_0 = 6.01 \), \( \Delta = 1.25 \) and \( U_0 = 0.422 \) a.u. \[3, 10\], or
\( r_0 = 5.262 \), \( \Delta = 2.9102 \), and \( U_0 = 0.2599 \) a.u. \[1, 3, 12\]
(originally suggested in \[12\]). A better choice of the pa-
rameters with an eye on \( e + C_{60} \) scattering was investi-
gated in Refs. \[4, 12\]. The made conclusion was in favor
of the latter set of parameters: \( r_0 = 5.262 \), \( \Delta = 2.9102 \),
and \( U_0 = 0.2599 \) a.u. This is because the chosen set of pa-
rameters leads to a better agreement between some of the
most prominent features of \( e + C_{60} \) elastic scattering pre-
dicted by the described model and the sophisticated \( ab
initio \) static multiconfigurational Hartree-Fock approxi-
mation \[12\]. Correspondingly, in the present work, \( U_c(r) \)
potential is defined by \( \Delta = 2.9102 \), \( r_0 = 5.262 \), and
\( U_0 = 0.2599 \) a.u.

B. Polarizable \( A@C_{60} \)

1. Polarizable \( A \) but “frozen” \( C_{60} \)

Let us first account for the impact of dynamical polari-
zation of only an atom \( A \), encapsulated inside \( C_{60} \), on \( e + A@C_{60} \) elastic scattering. This should help,
later in the paper, to appreciate the importance of the
effect of \( C_{60} \) polarization, in addition to that of \( A \), on
\( e + A@C_{60} \) scattering, to finalize the study.

In the present work, as in Ref. \[3\], the impact of polariza-
tion of \( A \) on \( e + A@C_{60} \) scattering (where the \( C_{60} \) cage is
“frozen”) is accounted on the first-principle basis by
utilizing the concept of the self-energy part of the Green’s function of an incident electron \[6, 7\]. In the simplest second-order perturbation theory in the Coulomb interelectron interaction \(V\) between the incident and atomic electrons, the irreducible self-energy part of the Green’s function \(\Sigma(\epsilon)\) of the incident electron is depicted with the help of Feynman diagrams in Fig. [1]

![Diagram](image)

FIG. 1. The irreducible self-energy part \(\Sigma(\epsilon)\) of the Green function of a scattering electron in the second-order perturbation theory in the Coulomb interaction, referred to as the SHIFT approximation (see text). Here, a line with a right directed arrowhead denotes either scattered states \(|\epsilon\rangle\) and \(|\epsilon'\rangle\), or atomic excited states \(|m\rangle\), a line with a left directed arrowhead denotes the states \(|j\rangle\) and \(|\ell\rangle\) of a vacancy (hole) in the atom, and a wavy line denotes the Coulomb interelectron interaction \(V\).

The diagrams of Fig. 1 illustrate how a scattered electron “\(\epsilon''\)” polarizes a \(j\)-subshell of the atom by causing \(j \rightarrow m\) excitations from the subshell and couples with these excited states itself via both the Coulomb direct [diagrams (a) and (b)] and exchange [diagrams (c) and (d)] interactions. Numerical calculations of electron elastic-scattering phase shifts, in the framework of this approximation, are performed with the help of the computer code from Ref. [7] labeled as “SHIFT”. Correspondingly, the authors refer to this approximation as the “SHIFT” approximation everywhere in the present paper.

A fuller account of the effect of the encapsulated-atom polarization in \(e + A\text{C}_{60}\) elastic scattering is determined by the reducible \(\Sigma(\epsilon)\) part of the self-energy part of the electron’s Green function [3]. The matrix element of the latter are represented diagrammatically in Fig. [2]

![Diagram](image)

FIG. 2. The matrix element of the reducible self-energy part \(\tilde{\Sigma}(\epsilon)\) of the Green’s function of a scattering electron, where \(\Sigma\) is the irreducible self-energy part of the Green’s function depicted in Fig. [1]. This approximation is referred to as the SCAT approximation (see text). Note, when calculating \(\langle \epsilon_\ell | \tilde{\Sigma} | \epsilon_\ell \rangle\) analytically, the summation over unoccupied discrete and integration over continuum excited states (marked as \(\epsilon''\)) along with the summation over the occupied states in the atom marked as \(E_{\text{el}}\) must be performed.

works well for the case of electron scattering off free atoms [3]. This gives us confidence in that SCAT is a sufficient approximation for pinpointing the impact of correlation/polarization of \(A\text{C}_{60}\) electrons on \(e + A\text{C}_{60}\) scattering as well.

In the framework of SHIFT or SCAT, the electron elastic-scattering phase shifts \(\zeta_\ell\) are determined as follows [7]:

\[
\zeta_\ell = \delta_\ell^{\text{HF}} + \Delta \delta_\ell. \tag{6}
\]

Here, \(\Delta \delta_\ell\) is the correlation/polarization correction term to the calculated HF phase shift \(\delta_\ell^{\text{HF}}\) [7]:

\[
\Delta \delta_\ell = \tan^{-1}(-\pi \langle \ell \ell | \tilde{\Sigma} | \ell \ell \rangle). \tag{7}
\]

The mathematical expression for \(\langle \ell \ell | \tilde{\Sigma} | \ell \ell \rangle\) is cumbersome. The interested reader is referred to [7] for details. The matrix element \(\langle \ell \ell | \tilde{\Sigma} | \ell \ell \rangle\) becomes complex for electron energies exceeding the ionization potential of the atom-scatterer, and so does the correlation term \(\Delta \delta_\ell\) and, thus, the phase shift \(\zeta_\ell\) as well. Correspondingly, \(\zeta_\ell = \delta_\ell + i \mu_\ell\) or

\[
\delta_\ell = \delta_\ell^{\text{HF}} + \text{Re} \Delta \delta_\ell, \quad \mu_\ell = \text{Im} \Delta \delta_\ell. \tag{9}
\]

The total electron elastic-scattering cross section \(\sigma_{\text{el}}\) is then given by the expression

\[
\sigma_{\text{el}} = \sum_{\ell = 0}^{\infty} \sigma_\ell, \tag{10}
\]

where \(\sigma_\ell\) is the electron elastic-scattering partial cross section [7]:

\[
\sigma_\ell = \frac{2\pi}{k^2} (2\ell + 1) \cosh 2\mu_\ell - \cos 2\delta_\ell e^{-2\mu_\ell}. \tag{11}
\]
2. Polarizable $A$ and $C_{60}$: approximation of “uncoupled” polarizabilities

We now account for the effects of polarization of $C_{60}$ by an incoming electron in addition to the encapsulated atom polarization. This is done in a simple approximate way, as is often done in atomic physics [12]. Namely, the long-range polarization potential of $C_{60}$ is approximated by a static dipole polarization potential $V_p(r)$:

$$V_p(r) = -\frac{\alpha}{2(r^2 + b^2)^{2}}. \quad (12)$$

Here, $\alpha$ is the static dipole polarizability of $C_{60}$ and $b$ is the “cut-off” parameter of the order of the radius of $C_{60}$, $r_0$.

In the present work, the $C_{60}$ effective potential $V_{C_{60}}^{\text{eff}}(r)$, “felt” by an incident electron, is approximated by the sum of the short-range potential $U_c(r)$, Eq. (1), and the long-range polarization potential $V_p(r)$, Eq. (12):

$$V_{C_{60}}^{\text{eff}}(r) = U_c(r) + V_p(r). \quad (13)$$

In the given approximation, the wavefunctions of the ground and excited states of the atom $A$ are calculated with the help of Eq. (2), where the potential $U_c(r)$ is replaced by $V_{C_{60}}^{\text{eff}}(r)$. Such defined wavefunctions are used in calculations of $e+A@C_{60}$ elastic-scattering phase shifts with account for dynamical polarization of the atom $A$ in the presence of polarizable $C_{60}$. This is done in the framework of the above described Dyson formalism for the self-energy part of the Green function of an incident electrons, Eqs. (5)-(11). The determined phase shifts are plugged into Eqs. (5) and (7) to meet the goal of the study, that is to account for the impact of both dipole static polarization of $C_{60}$ (in the model approximation) and dynamical polarization of the encapsulated atom $A$ (on the first-principle basis) on $e+A@C_{60}$ scattering.

In the developed approximation, the polarizabilities of $C_{60}$ and $A$ are, obviously, not coupled with each other (no interelectron interaction between the electrons of $A$ and $C_{60}$). This approximation is referred to as the approximation of “uncoupled” polarizabilities of $C_{60}$ and $A$ in the present paper.

3. Polarizable $A$ and $C_{60}$: approximation of “coupled” polarizabilities

In the present paper, the term “coupled polarizabilities” of $A$ and $C_{60}$ means coupling between excited configurations of $A$ and $C_{60}$, both of which are caused by an incident electron. The corresponding correction to $e+A@C_{60}$ scattering is in addition to the above discussed effect of “uncoupled” polarizabilities of $A$ and $C_{60}$. In the present work, this is done, first, by adding some specific third order terms of perturbation theory in Coulomb interaction to the irreducible $\Sigma(\epsilon)$ (Fig. 4). Then, thus re-defined $\Sigma(\epsilon)$ is substituted into the equation for the reducible part of the Green function $\Sigma(\epsilon)$ [Eq. (5)] and/or

![FIG. 3. The multielectron processes accounting for the interaction between excited configurations of $C_{60}$ and $A$ brought about by an incident electron. Lines marked as “$C_{60}$” and “$m$” denote the core and excited states of the fullerene cage $C_{60}$, respectively. Other notations are the same as in Fig. 1](image-url)

Strictly speaking, to calculate the terms depicted in Fig. 2 one needs to calculate wavefunctions of the ground and excited states of the multielectron fullerene cage $C_{60}$. In the present paper, we bypass this difficulty by employing a simple and yet reasonable approximation. It is consists in the following. First, it takes into account that the radius $r_0$ of the $C_{60}$ cage is bigger than the radius $r_A$ of an encapsulated atom $A$: $r_0 > r_A$. Second, it exploits the fact that the impact of the polarization potential of $C_{60}$ on electron scattering is essential only at large distances $r_p$ from the target. Hence, $r_p > r_0$, $r_p$ being the important electron-projectile distance from the center of $C_{60}$. Next, as a not too strong exaggeration, let us regard that $r_p \gg r_0 \gg r_A$. Then, the Coulomb interaction between the incident electron and $C_{60}$’s electrons, $V(r_p, r_C) \propto |r_p - r_C|^{-1}$, and that one between the $C_{60}$’s electrons and electrons of the encapsulated atom $A$, $V(r_A, r_C) \propto |r_A - r_C|^{-1}$, turn, approximately, into the long-range dipole potentials:

$$V(r_p, r_C) \propto \frac{r_p r_C}{r_p^3}, \quad V(r_A, r_C) \propto \frac{r_A r_C}{r_C^3}. \quad (14)$$

Hence, the exact Coulomb interactions, represented by the first and second wavy lines in the diagrams of Fig. 3 can now be replaced by their approximate values defined by Eqs. (14). This is equivalent to accounting for the impact of only dipole polarization of $C_{60}$ on electron scattering. The impact can be expressed via the known dipole polarizability $\alpha$ of $C_{60}$, similar to how it has been done in
Ref. [15]. One can show that this is equivalent to making simple replacements
\[
|V|^2 \rightarrow |V[1 - \alpha (\epsilon_\ell - \epsilon_\ell')/r_0^3]|^2
\] (15)
in the diagrams (a) and (c) of Fig. [1] and
\[
|V|^2 \rightarrow |V[1 - \alpha (\epsilon_\ell - \epsilon_\ell')/r_0^3]| \times V[1 - \alpha (\epsilon_\ell - \epsilon_m)/r_0^3].
\] (16)
in the diagrams (c) and (d) of Fig. [1]. Next, the recalculated \( \Sigma(e) \) (Fig. [1]) is substituted into Eq. (5) for \( \Sigma(e) \). The latter concludes the problem of \( e + A@C_{60} \) scattering in the framework of the approximation of coupled polarizabilities of \( C_{60} \) and \( A \).

III. RESULTS AND DISCUSSION

A. Preliminary notes

First, in order the modeling of the \( C_{60} \) cage by the homogeneous spherical potential \( U_c(r) \), Eq. (1), made sense, the wavelength \( \lambda \) of an incident electron must exceed greatly the bond length \( D \approx 1.44 \) \( \text{Å} \) between the carbon atoms in \( C_{60} \). In the present work, therefore, the maximum energy of an incident electron is capped at approximately 4 eV. Up to this energy, \( \lambda \gtrsim 6 \) \( \text{Å} \), so that, indeed, \( \lambda \gg D \).

Second, given that the outer radius of \( C_{60} \) is approximately 8 a.u., one can easily estimate that the maximum contribution to electron scattering comes from the first five electron partial waves with \( \ell \) ranging from 0 to 4. Correspondingly, in the present work, the maximum value of \( \ell \) is capped at \( \ell = 4 \).

Third, when accounting for multipolar excitations of the electronic subshells of an encapsulated atom \( A \) by an incident electron, the performed calculations accounted for the monopole, dipole, quadrupole, and octupole excitations of outer subshells of the atoms. For the chosen in the present paper set of encapsulated atoms, these are the \( 6s^2 \) and \( 5p^6 \) subshells in \( Ba \), \( 5p^6 \) in \( Xe \), and \( 2p^6 \) in \( Ne \).

Fourth, since one of the main goals of this study is to explore how both the size of an atom and its dynamical polarizability might affect electron scattering off polarizable \( A@C_{60} \), the study is run along the path from the most compact to the most diffuse encapsulated atom: \( e + Ne@C_{60} \rightarrow e + Xe@C_{60} \rightarrow e + Ba@C_{60} \).

Finally, in order to facilitate the reader to cope with various abbreviations for the utilized approximations, adopted in the present paper, these are as follows:

- **HF** stands for the model static HF approximation, where both the encapsulated atom \( A \) and the fullerene cage \( C_{60} \) are regarded as non-polarizable targets (see subsection A above).
- **SCAT(A@)** marks the approximation, which accounts for polarization of only the encapsulated atom \( A \) (see subsection 1 of subsection B).
- **SCAT(A)** designates the approximation as the above one, but in relation to a free atom \( A \).
- **SCAT(UP)** labels the approximation of uncoupled polarizabilities of \( C_{60} \) and \( A \) (see subsection 2 of subsection B).
- **SCAT(CP)** stands for the approximation of coupled polarizabilities of \( C_{60} \) and \( A \) (see subsection 3 of subsection B).

B. \( e + Ne@C_{60} \) scattering

Based on our previous HF calculated data for \( e + A@C_{60} \) scattering [1, 3], it is known that the encapsulation of \( Xe \) into the \( C_{60} \) cage practically does not change electron elastic scattering off \( e + A@C_{60} \) compared to scattering by empty \( C_{60} \) calculated within the model static approximation. This is because the \( Xe \) atom is compact. Obviously, one can expect the same for even smaller compact atoms, like the \( Ne \) atom. In addition, the \( Ne \) atom has a smaller polarizability \( \alpha \) than that of \( Xe \) or \( Ba \). For example, experimental values of the static dipole polarizabilities of the ground states of \( Ne \), \( Xe \), and \( Ba \) are as follows: \( \alpha(\text{Ne}) \approx 2.67 \), \( \alpha(\text{Xe}) \approx 27.34 \), and \( \alpha(\text{Ba}) \approx 269 \) a.u. [16]. Therefore, the study of \( e + Ne@C_{60} \) scattering makes a particular sense in two respects. First, it allows to understand better how accounting for polarization of only \( C_{60} \) affects electron elastic scattering off \( C_{60} \) doped with a compact static atom. Second, the study can shed light on whether the coupling between the weak polarizability of a compact atom \( A \) with the large polarizability of \( C_{60} \) (\( \alpha \approx 850 \) a.u. [15]) can have a noticeable effect on \( e + A@C_{60} \) scattering compared to that calculated in the SCAT(UP) approximation. Common sense suggests that the effect should be negligible. However, as one of key findings of the present work, such intuitive perception turns out to be not entirely correct.

Calculated HF, SCAT(A@), SCAT(A), SCAT(UP), and SCAT(CP) data for the real parts \( \delta_\ell(e) \) of phase shifts, as well as the partial \( \sigma_\ell(e) \) and total \( \sigma_{el}(e) \) cross sections of a \( e + Ne@C_{60} \) elastic collision are displayed in Fig. [4].

One can see that the difference between calculated model static HF data and SCAT(A@) data for all partial electronic waves is negligible. This agrees with common sense, in view of insignificant polarizability of \( Ne \). The data also demonstrate that the polarizability of a free small-sized compact atom, like \( Ne \), remains small upon its encapsulation inside \( C_{60} \). Indeed, in the opposite case, the difference between calculated static HF and SCAT(A@) data would have been noticeable.

Let us now explore the calculated data for the \( p-, d-, f-, \) and \( g- \) partial electronic waves scattered off \( Ne@C_{60} \). One can conclude that simultaneous accounting for polarization of both \( Ne \) and \( C_{60} \) by the scattered electron [SCAT(UP) and SCAT(CP) approximations; dash and
solid lines, respectively] has a huge effect on the corresponding cross sections compared to when only polarization of Ne is accounted [SCAT(A[@]), dash-dot line]. This was expected in view of a large polarizability of C60. Yet, details of how the polarization of C60 affects e + A@C60 scattering have been cleared up only in the present study, to the authors’ best knowledge. Next, one can also see that the effect of coupling between the polarizabilities of Ne and C60 [SCAT(CP) approximation, solid line] on scattering of these partial electronic waves off e + Ne@C60 is insignificant. Indeed, the calculated SCAT(CP) and SCAT(UP) (dash line) data are practically identical. This, again, fits common sense, in view of a small polarizability of Ne.

However, the study finds that s-scattering behaves quite differently compared to the above case of scattering of waves with higher ℓs. In contrast to the above case, we found both big quantitative and qualitative differences between calculated σs^{SCAT(UP)} (dash line) and σs^{SCAT(CP)} (solid line). Indeed, σs^{SCAT(UP)} is seen to monotonically increase, whereas, in contrast, σs^{SCAT(CP)} develops a strong maximum with decreasing electron energy ϵ. The reason for the different behavior of σs^{SCAT(CP)} versus σs^{SCAT(UP)} becomes clear upon exploring the corresponding phase shifts. One can see that the phase shift δs^{SCAT(CP)} (solid line on inset) crosses the value of modulo π/2 at ϵ → 0, whereas δs^{SCAT(UP)} (dash line on inset) does not. Correspondingly, the cross section σs^{SCAT(CP)} develops a shape resonance at low ϵ, in opposition to σs^{SCAT(UP)}. Note, the behavior of the phase shift δs^{SCAT(CP)} speaks to the fact that the binding potential of e + Ne@C60 gets stronger when the polarizabilities of Ne and C60 are coupled. This results in the emergence of an additional bound s-state in the field of e + Ne@C60 (compared to the approximation on uncoupled polarizabilities), thereby pushing δs^{SCAT(CP)} to a larger value than that of δs^{SCAT(UP)}, at ϵ → 0. This is in accordance with the well known Levinson theorem: δℓ → nℓπ at ϵ → 0, nℓ being the total number of bound ℓ-states in the system (valid when projectile-target electron exchange is neglected, as in the present work).

Another interesting effect relevant to s-scattering is that coupling between polarizabilities of C60 and Ne is found to largely cancel out the strong polarization impact of C60 on σs^{Ne@C60} in a broad energy region to the right of the maximum in σs^{SCAT(CP)} (solid line). Indeed, there, σs^{SCAT(CP)} differs only somewhat from both σs^{HF} (dash-dot-dot line) and σs^{SCAT(A[@])} (dash-dot line), but it differs significantly from σs^{SCAT(UP)} (dash line). We, thus, have unraveled an interesting effect. Namely, it is found that coupling of the large polarizability of C60 with the considerably smaller polarizability of a compact encapsulated atom can have a significant impact on scattering of at least some of electronic partial waves off A@C60. This, in turn, affects the total electron elastic scattering cross section σ_\text{tot}^{A@C60} as well, in the corresponding regime of electron energies (cp. dash and solid lines in the right bottom panel of Fig. 4).

Next, we comment on one more interesting finding related to scattering of a g-partial electronic wave. The g-wave is seen to induce a strong narrow resonance in the g-partial scattering cross section σg of e + Ne@C60 scattering. The resonance is predicted by each of the utilized approximation: HF, SCAR(A[@]), SCAT(UP), and SCAT(CP). The origin of this resonance in g-scattering was established earlier in Refs. [4, 12], where it was shown that this is a shape resonance. One can see that the resonance in the cross section σg, calculated both in SCAT(UP) and SCAT(CP) approximations, emerges at noticeably lower energies and becomes significantly narrower than that in σg calculated in the framework of HF or SCAR(A[@]). The emphasized difference is interesting. The fact that the g-resonance emerges at the lowest
energy and is the most narrow when calculated in the SCAT(CP) framework means that coupling between polarizabilities of C_{60} and A can result in a much stronger binding potential of A@C_{60} than that calculated otherwise.

Lastly, the performed calculations demonstrate that accounting for polarization of A@C_{60} by a scattered electron results in the emergence of near-zero minima in all partial cross sections \(\sigma_s\). We refer to these minima as the Ramsauer minima by analogy with the known Ramsauer minima in electron elastic-scattering cross sections of some of free atoms (e.g., Xe). The presence of Ramsauer minima in all \(\sigma_s\) for e + Ne@C_{60} scattering might prompt one to conclude that the total scattering cross section \(\sigma_{tot}^{Ne@C_{60}}\) could be so small that it might fall below the electron elastic-scattering cross section of free Ne, \(\sigma_{tot}^{Ne}\), at some electron energy. This, however, does not happen, because Ramsauer minima in the partial cross sections \(\sigma_s^{Ne@C_{60}}\) for different \(\ell_s\) emerge at somewhat different energies. Therefore, the minimum value of the total cross section \(\sigma_{tot}^{Ne@C_{60}}\) remains far greater than the cross section \(\sigma_{tot}^{Ne}\). In the present case, \(\sigma_{tot}^{Ne@C_{60}}\) \(\approx\) 60 a.u. at \(\epsilon \approx 1.4\) eV, whereas the electron elastic-scattering cross section of free Ne is one order of magnitude smaller, \(\sigma_{tot}^{Ne} \approx 6\) a.u., at 1.4 eV (cp. a solid or a dash line with a dot line in right bottom panel of Fig. [5]).

C. \(e + Xe@C_{60}\) scattering

We next explore changes in \(e + A@C_{60}\) scattering with increasing size and polarizability of an encapsulated atom \(A\) which, however, is still a relatively compact atom of moderate polarizability. To meet the goal, we study \(e + Xe@C_{60}\) scattering. Corresponding calculated data are displayed in Fig. [5]

Overall important similarities in, and difference between \(e + Xe@C_{60}\) and \(e + Ne@C_{60}\) scattering surface upon comparison of Fig. [5] with Fig. [4]

We start focusing on similarities in \(e + Xe@C_{60}\) and \(e + Ne@C_{60}\) scattering. The overall impact of polarization of Xe@C_{60} by an incident electron on \(e + Xe@C_{60}\) scattering remains significant. It results in the corresponding partial and total cross sections that differ strongly from those calculated without regard for the polarization effect. Next, similar to s-scattering off Ne@C_{60}, the effect of coupled polarizabilities of Xe and C_{60} [SCAT(CP) approximation] impacts strongly the s-scattering cross section. Indeed, this impact results in a strong shape resonance in \(\sigma_{s}^{SCAT(CP)}\) (solid line) below 1 eV of the electron energy. Furthermore, when coupling between polarizabilities of Xe and C_{60} is accounted in the calculation of s-scattering, it largely cancels out the overall polarization impact of Xe@C_{60} on s-scattering in a broad energy region to the right of the maximum in \(\sigma_{s}^{SCAT(CP)}\) (solid line). Indeed, there, the s-cross section becomes about the same as the one calculated in the SCAT(A@) and HF approximations (dash-dot and dash-dot-dot lines). The emergence of the noted cancelation effect in two independent calculations – s-scattering off Xe@C_{60} and off Ne@C_{60} – speaks to the fact that the discovered effect is not accidental. Next, coupling between polarizabilities of Xe and C_{60} results in the emergence of Ramsauer minima in corresponding \(\sigma_s\). Lastly, similar to \(e + Ne@C_{60}\) scattering, the total cross section \(\sigma_{tot}^{Xe@C_{60}}\) exceeds noticeably that for electron scattering off free Xe (note, the cross section of electron elastic scattering off free Xe has its own low-energy Ramsauer minimum as well, in contrast to that for Ne).

The most striking differences between \(e + Xe@C_{60}\) and \(e + Ne@C_{60}\) scattering consist in the following. First, in contrast to a \(d\)-wave scattering off Ne@C_{60}, the \(d\)-wave scattering off Xe@C_{60} is subject to a particularly strong impact of coupled polarizabilities of Xe and C_{60}. Indeed, in the present case, the \(d\)-scattering cross section \(\sigma_d^{SCAT(CP)}\) (solid line) develops the intense shape resonance below of 1 eV and differs qualitatively and quantitatively from calculated data obtained in the frame-
works of the SCAT(UP) (dash line) and other utilized approximations. Second, the overall differences between calculated SCAT(UP) and SCAT(CP) electron scattering cross sections (both partial and total) are noticeably stronger in the case of \(e + \text{Xe@C}_{60}\) scattering than in \(e + \text{Ne@C}_{60}\) scattering.

In summary, the highlighted differences between \(e + \text{Xe@C}_{60}\) and \(e + \text{Ne@C}_{60}\) underpin the effect of a bigger size and greater polarizability of a compact encapsulated atom \(A\) on \(e + A@\text{C}_{60}\) scattering.

D. \(e + \text{Ba@C}_{60}\) scattering

In the earlier study of \(e + \text{Ba@C}_{60}\) scattering, the impact of the polarization of only encapsulated \(\text{Ba}\) on the scattering process was accounted in the calculations [the SCAT(A@) approximation]. This impact was found to be considerable, due to a large value of the \(\text{Ba}\) polarizability. The \(e + \text{Ba@C}_{60}\) scattering, therefore, stands out of the cases of \(e + \text{Ne@C}_{60}\) and \(e + \text{Xe@C}_{60}\) scattering. It sheds light on features of the impact of coupled polarizabilities of a highly-polarizable atom and highly-polarizable \(\text{C}_{60}\) on \(e + A@\text{C}_{60}\) scattering. Corresponding calculated data for \(e + \text{Ba@C}_{60}\) scattering are displayed in Fig. 6.

An interesting feature, which caught our attention in the first head, is a cancelation effect of a new quality in the scattering process, compared to electron scattering off \(\text{Ne@C}_{60}\). For higher \(\ell\) approximation. For higher \(\ell\) compared to electron scattering the first head, is a cancelation effect of a new quality in the scattering process, compared to electron scattering off \(\text{Ne@C}_{60}\). The \(e + \text{Ba@C}_{60}\) scattering, therefore, stands out of the cases of \(e + \text{Ne@C}_{60}\) and \(e + \text{Xe@C}_{60}\) scattering. It sheds light on features of the impact of coupled polarizabilities of a highly-polarizable atom and highly-polarizable \(\text{C}_{60}\) on \(e + A@\text{C}_{60}\) scattering. Corresponding calculated data for \(e + \text{Ba@C}_{60}\) scattering are displayed in Fig. 6.

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The reader can spot a number of other impressive differences between \(\sigma_{g}\), or between \(\sigma_{g\ell}\) for \(e + \text{Ba@C}_{60}\) scattering calculated in each of the utilized approximations, and/or between calculated data for \(e + \text{Ba@C}_{60}\) scattering, on the one hand, and \(e + \text{Ne@C}_{60}\) and \(e + \text{Xe@C}_{60}\) scattering, on the other hand.

In summary, similar to the earlier commentary on the differences between electron scattering off \(\text{Ne@C}_{60}\) and \(\text{Xe@C}_{60}\), the highlighted features of electron scattering off \(\text{Ba@C}_{60}\) underpin, on a bigger scale, the effect of a greater size and polarizability of a compact encapsulated atom \(A\) on \(e + A@\text{C}_{60}\) scattering.

FIG. 6. (Color online) Main panels: Calculated partial \(\sigma_{g}(\ell)\) and total \(\sigma_{g}(\ell)\) cross sections (in atomic units) for electron elastic scattering off \(\text{Ba@C}_{60}\). Insets: Real parts \(\delta_{g}(\ell)\) of the phase shifts (in units of radian); \(\mu_{e} = 0\) in this energy region. The used styles of the plotted lines mark results obtained in different approximation utilized in the present work, as follows: dash-dot-dot, HF; dash-dot, SCAT(A@); dash, SCAT(UP); solid, SCAT(CP) (the most complete approximation).

IV. CONCLUSION

The present work provides the wealth of information about the role and significance of various polarization effects in \(e + A@\text{C}_{60}\) scattering unraveled in the framework of reasonably simple approximations developed and utilized in the present work.

As of today, this study provides the most complete information about features of \(e + A@\text{C}_{60}\) scattering brought about by various confinement-related, static-related, and dynamical-related impacts of individual and coupled “members” of \(A@\text{C}_{60}\) on electron elastic scattering off this complex target. Each of these impacts has been found to bring specific features into \(e + A@\text{C}_{60}\) scattering. Spectacular effects in the scattering process, primarily associated with polarization of \(A@\text{C}_{60}\) by an incident electron have been unraveled, scrutinized, and fully detailed in this paper in a physically transparent manner.

The overall conclusion is that not only the individual impacts of uncoupled polarizabilities of the encapsulated atom \(A\) (especially of a highly-polarizable atom) and \(C_{60}\)
on $e + A@C_{60}$ scattering are generally important, but the correction term to $e + A@C_{60}$ scattering, brought about by coupled polarizabilities of the atom $A$ and $C_{60}$, is essential. The significance of its impact on $e + A@C_{60}$ scattering is found to increase with increasing size and polarizability of the atom $A$. For example, the effect of coupled polarizabilities of Ba and $C_{60}$ was demonstrated to result in considerable quantitative and qualitative modifications of partial cross sections for $e + Ba@C_{60}$ scattering at lower energies, whereas it was found to largely annihilate the whole polarization impact on scattering of $s$, $p$, $d$, and $f$-partial waves above $\epsilon \approx 1.4eV$.

The authors hope that the present work will prompt other theorists to perform more rigorous calculations of $e + A@C_{60}$ scattering. However, in the absence of experimental data on the subject, the question of which theory is most appropriate to meet the goal would remain an open one. This should prompt experimentalists to perform corresponding measurements as well.

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