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Elastic electron scattering from $Ar@C_{60}^{z+}$: Dirac-partial wave analysis

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Abstract

Photoionization spectra of $A@C_{60}^{z-}$ introduces interesting features like Coulomb confinement resonances (CCR); a new variety of confinement resonances caused due to Coulomb barrier, whereas for cationic states merely a shift of ionization potential towards higher threshold is noticed [1]. It is imperative to search for the electron scattering dynamics with such targets, which is not elaborately explored so far compared to that of neutral targets [2-3]. The present work accounts for a detailed analysis of scattering parameters using Dirac partial wave analysis, emphasizing the role of encaged Ar atom and C_{60}^{z+} cage in electron scattering from $Ar@C_{60}^{z+}$ for z=1 and 6. Two contrasting types of model C_{60} potential with charged-shell potential are employed [1]. The role of Coulomb field and short-range interactions on scattering dynamics is elucidated through an analysis of the non-Coulomb scattering phase shifts. Differential cross section shows (DCS) oscillatory structures owing to interference of Coulomb and short-range interactions at the intermediate angles. DCS at backward angles comprises of interferences arising due to internal structure of the target (short-range field) [4] and Coulomb field dominates near the forward angles. A piecewise scattering approximation can be proposed for charged endohedral scattering, similar to the way it was introduced earlier in electron scattering with endohedral target [2]. Total cross section shows solely the dominance of Coulomb field; irrespective of the size of target. Target polarization is found significant for smaller z and at low energy.

Introduction

Owing to the favorable modifications of intrinsic properties of isolated molecules and atoms, a major focus of the modern research is on investigations of structure and dynamics of confined systems. Since the pathbreaking discovery of C_{60} by Kroto et al. [5], there has been series of theoretical and experimental studies on them in various fields of technological and fundamental importance. Potential applications of the C_{60} which attracted the attention of scientific community includes isolation of poisonous atoms and substances in medical imaging and cancer therapy [6], providing building block for the qubits of a quantum computer [7], an important constituent of the interstellar medium [8], hydrogen storage [9], etc. Atom/molecule or compound entrapped inside the C_{60} cage are called as endohedral species, denoted popularly as $A@C_{60}$ and the confined entities as @A. In order to explore such amazing systems dynamical study using scattering and photoionization tools is an essential demand.

There exist no detailed study for e-$A@C_{60}^{z}$ scattering dynamics, compared to sufficiently developed area of corresponding photoionization studies [1,10]. To accomplish this gap we report the elastic electron scattering from $Ar@C_{60}^{z+}$ targets with charge states z=1 and 6 as a case study. The reason behind choosing Ar as an encaged atom is two-fold. Primarily, rare gas C_{60} endohedrals ($Ar@C_{60}$) are found in nature. Secondly, being an inert gas, it is supposed to be located at the center of the C_{60}^{z+} cage as is assumed in earlier studies [1-2], which makes the theoretical calculations easier. In order to elucidate effect of presence of @Ar, we also calculate e-C_{60}^{z+} and e-Ar^{z+} scattering dynamics. The scattering problem is solved employing the Dirac partial wave analysis [11] in static-exchange approximation for @Ar including target polarization.

Theoretical methodology

The model potential for C_{60} molecule is given by two different nature of interactions: a compact annular square well (ASW) model [1-2] and a diffuse Gaussian annular square well (GASW) [12] model given as:

$$V_{ASW}(r) = \begin{cases} -U, & r_c - \frac{\Delta}{2} \le r \le r_c + \frac{\Delta}{2} \\ 0, & otherwise, \end{cases} \tag{1}$$

where $U = 0.2599\ a.u.$ is the well depth, radius $r_c = 6.7173\ a.u.$, and $\Delta = 2.9102\ a.u.$ is the C_{60}- cage width.

$$V_{GASW}(r) = \frac{A}{\sqrt{2\pi}\,\sigma} e^{-\left(\frac{(r-r_c)}{\sqrt{2}\sigma}\right)^2} + V_{ASW}(r), \tag{2}$$

where standard deviation $\sigma = 1.70\ a.u.$, and $\frac{A}{\sqrt{2\pi}\,\sigma} - U$ is the depth of the potential at $r = r_c$. U=0.1181 a.u. and $\frac{A}{\sqrt{2\pi}\,\sigma} = -0.1417$ a.u.

The charged-shell interaction of C_{60}^{z+} is given by:

$$V_z(r) = \begin{cases} \frac{z}{r_c+\Delta}, & if\ 0 \le r \le r_c + \Delta \\ \frac{z}{r}, & otherwise \end{cases}, \tag{3}$$

The target polarization for charged-C_{60} cage is given by:

$$V_{C_{60}^{z+}-pol}(r) = -\frac{\alpha_{C_{60}^{z+}}}{2(r^2+b^2)^2}. \tag{4}$$

For the encaged Ar atom exchange interaction is modelled by Furness-McCarthy exchange model, given as:

$$V_{ex}(r) = \frac{1}{2}[E - V_{st}(r)] - \frac{1}{2}\{[E - V_{st}(r)]^2 + 4\pi a_0 e^4 \rho(r)\}^{\frac{1}{2}}, \tag{5}$$

The polarization potential for encaged Ar is modelled by popular Buckingham potential. The total interaction hence can be given by:

$$V_T(r) = V_{st}(r) + V_{ex}(r) + V_{C_{60}}(r) + V_z(r) + V_{C60-pol}(r) + V_{@A-pol}(r). \tag{6}$$

Here $V_{st}(r)$ is electrostatic potential of encaged Ar. The scattering problem is solved by adapting the popular code package ELSEPA [13] to meet the needs of model and charged-shell potential of the C_{60}. The asymptotic form of the large component of radial wave function is :

$$P_{E\kappa}(r) \simeq \sin\left(kr - \ell\frac{\pi}{2} - \eta \ln 2kr + \Delta_\kappa\right), \tag{7}$$

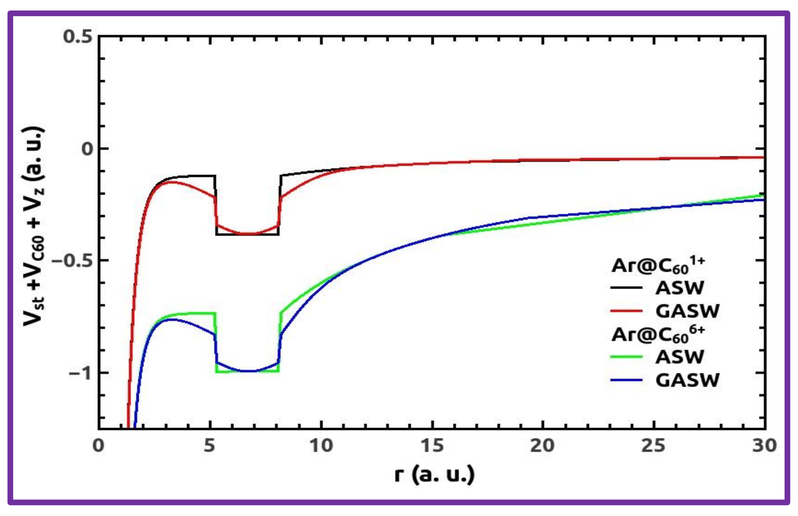
$$\Delta_\kappa = \Omega_\kappa + \delta_\kappa.$$

The first term in phase shift Δ_κ is Coulomb phase shifts and the second arises due to short range interaction of the target. These phase shifts are used to finally obtain the DCS and TCS for our scattering problem.

Results and Discussion

Subshells	Binding energy (a.u.)						
	Free Ar	$Ar@C_{60}^{z+}$					
		ASW			GASW		
		z=0	z=1	z=6	z=0	z=1	z=6
$1s_{1/2}$	119.126	119.132	119.255	119.866	119.147	119.270	119.881
$2s_{1/2}$	12.412	12.417	12.540	13.152	12.431	12.553	13.165
$2p_{1/2}$	9.632	9.638	9.760	10.372	9.651	9.774	10.386
$2p_{3/2}$	9.547	9.553	9.675	10.287	9.566	9.689	10.301
$3s_{1/2}$	1.286	1.291	1.413	2.025	1.300	1.422	2.034
$3p_{1/2}$	0.595	0.599	0.721	1.333	0.609	0.731	1.343
$3p_{3/2}$	0.588	0.591	0.714	1.326	0.601	0.723	1.335

Table 1: An overview of calculated binding energy of encaged Ar atom for charge states z=1 and 6. The free Ar atom subshell binding energies are also provided as a reference. Though the electronic distribution of encaged Ar remains same as free Ar.



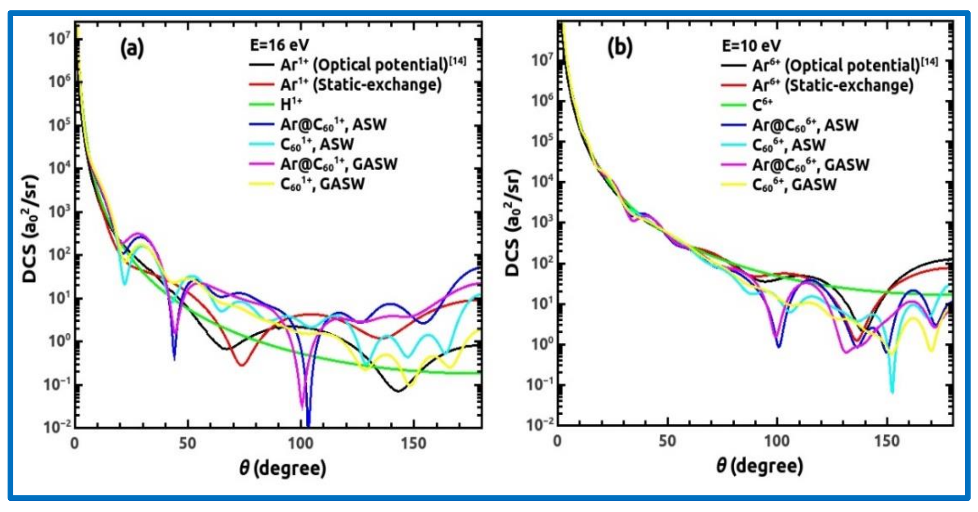
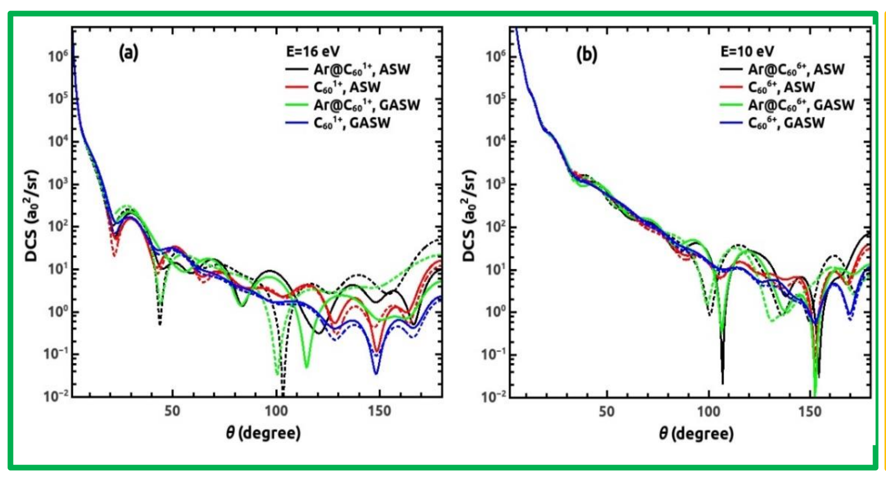


Fig. 1 (left panel) depicts the nature of projectile-target interaction marked by Coulomb field at large r and short-range interactions at small r. Fig. 2 (right panel) shows DCS for z=1 and 6 at E=16 and 10 eV respectively for various targets.



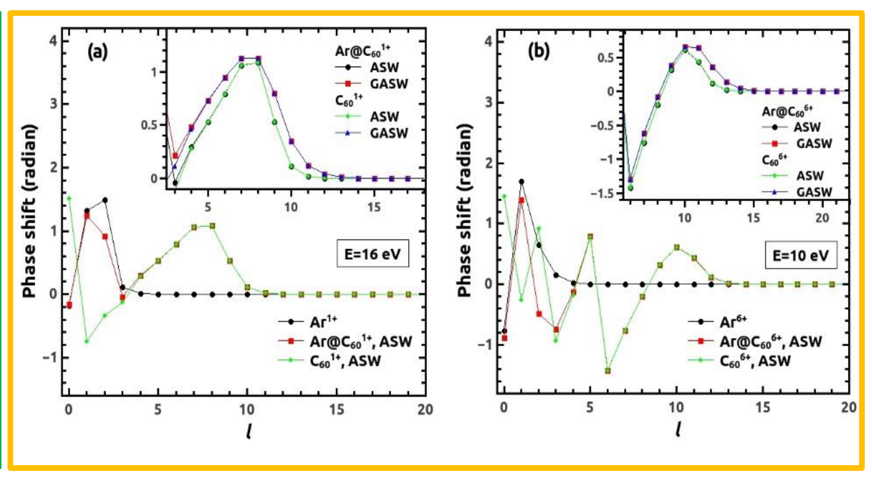


Fig. 3 (left panel) shows DCS for the same target and same energy after inclusion of polarization potential. Fig 4 (right panel) gives an account of the non-Coulomb scattering phase shifts for DCS plot shown in Fig. 2 above.

Conclusions

- ❖ Binding energy of the encaged atom is enhanced in proportional with the charge state z, a constant amount of increment is seen proportional to z.
- ❖ No alteration in electron density distribution in encaged Ar orbital is seen in the ground state.
- ❖ High-angle scattering can be used as a sensitive tool to elucidate interior of the target.
- ❖ DCS is marked by interference structures over higher angle sides, which alters by different confining potentials: ASW and GASW.
- ❖ Interplay between Coulomb and short-range field leads to interferences in the DCS.
- ❖ DCS as well as non-Coulomb phase shifts are dependent on charge state z of the C_{60} shell.
- ❖ Target polarization is significant only for smaller charge states z and lower projectile energies.
- ❖ An piecewise picture of collision can be proposed where lower ℓ encounters the field of Ar and those of higher ℓ feel the field of charged C_{60}; C_{60}^{z+}.
- ❖ TCS is dominated solely by Coulomb interaction giving a resonance less structure.

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