

Article

Single-Electron Capture in Collisions of Carbon Ions with Water Molecules

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Abstract

Single-electron capture in the collisions of carbon ions, C^{q+} ($q = 1-6$), with water molecules is theoretically investigated using the continuum distorted wave-eikonal initial state (CDW-EIS) formalism. The projectile–electron interaction is modeled using three different approaches to account for screening effects: (i) the Green–Sellin–Zachor (GSZ) potential, which combines long-range Coulomb and short-range screening terms; (ii) a modified GSZ- Z_p^r variant employing an effective radius-dependent nuclear charge; and (iii) the binding energy screening (BES) approximation, which treats the projectile as a rigid Coulomb core. Total cross-sections for single-electron capture are computed over the energy range of 40 keV/u to 10 MeV/u. A detailed analysis is presented as a function of the initial molecular orbital, the final bound state of the captured electron, and the projectile charge state q . The results reveal strong dependencies on orbital binding energies and the degree of projectile ionization. Additionally, of radiobiological interest, the average binding energy for the different projectiles are computed using the presented cross-sections and reported.

Keywords: electron capture; water; carbon ions

1. Introduction

The study of electronic processes in ion–molecule collisions is highly relevant to a wide range of fields, including plasma physics, astrophysics, medical physics, and radiobiology. Electron capture by bare projectiles (e.g., H^+ , He^{2+} , C^{6+}) has been extensively studied [1], with numerous theoretical works reporting total cross-sections (TCSs) for charge transfer between highly charged bare ions and atomic or molecular targets. In particular, studies on ion-induced processes have focused on water molecules due to their significant relevance in radiobiological applications. In most contexts, water is considered a reliable surrogate for biological tissue, as living cells are primarily composed of water.

For collision energies above 10 keV/u, various theoretical models have been employed to investigate ionization and electron capture in collisions of bare projectiles with water and DNA/RNA molecules. These include the classical trajectory Monte Carlo (CTMC) method [2] and the perturbative continuum distorted wave (CDW) approximation [3–5]. Recently, the distorted wave (DW) approximation has also been used to investigate ionization processes in several biological targets [6]. Furthermore, non-perturbative approaches such as the two-center basis generator method (TC-BGM) have been applied to describe electron removal in collisions of H^+ , He^+ , and Li^{3+} with H_2O [7,8]. Subsequently, time-dependent CTMC calculations were performed to investigate electron processes in collisions of Li^{3+}



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and C^{3+} with water [9]. Additionally, cross-section predictions using the CTMC method with dynamic screening have been reported for various biological targets [10]. Collisions of highly charged projectiles with water were investigated by Otranto et al. using the CTMC method to compute state-selective electron capture cross-sections for ions with $Z_p = 4\text{--}26$ in the energy range of 1 to 100 keV/u [11]. Finally, motivated by the scarcity of data relevant to radiobiological applications such as hadron therapy, Liamsuwan and Nikjoo calculated cross-sections for electron removal in collisions of carbon ions with water molecules. They investigated these processes using the three-body CTMC method for projectiles in charge states $q = 1\text{--}6$ over an energy range from 1 to 1000 keV/u [12].

Several experimental results are available in the literature for proton-induced ionization processes on water molecules [13–17]. Measurements for helium ions impacting biological targets have also been reported [18,19]. Later, both experimental measurements and theoretical cross-sections for single- and multiple-electron removal from water molecules by bare Li^{3+} impact were reported [8]. Moreover, experimental data on electron capture by highly charged dressed ions are largely limited to the low-energy regime (below 10 keV/u) for molecular targets of biological interest. Absolute cross-sections for single charge exchange have been measured for C^{q+} , N^{q+} , O^{q+} , and Ne^{q+} ions impacting molecules such as H_2O , CO , and CO_2 at energies of a few keV/u [20,21]. Montenegro et al. studied water fragmentation induced by neutral and singly charged carbon projectiles (C^0 and C^+) [22], while Bodewits et al. used photon emission spectroscopy to measure final state-selective cross-sections for $O^{6+} + H_2O$ collisions in the 0.1–7.5 keV/u range [23]. Experimental measurements at intermediate collision energies (above a few tens of keV/u) remain scarce in the literature. Luna et al. investigated fragmentation cross-sections of H_2O induced by C^{3+} and O^{5+} ions [24], while, more recently, Maurya et al. reported data on single- and multiple-electron capture for 100 keV/u C^{4+} ions colliding with water molecules [17].

In the present work, we investigate single-electron capture from water molecules by C^{q+} projectiles ($q = 1\text{--}6$) in the intermediate- to high-energy range (40 keV/u to 10 MeV/u), a regime of direct relevance to carbon ion therapy applications. The process is treated within the continuum distorted wave-eikonal initial state (CDW-EIS) approximation, following the approach reported in [25]. The screening effects in the projectile–electron interaction are modeled using three different approaches: (i) the Green–Sellin–Zachor (GSZ) potential, which combines long-range Coulomb and short-range screening terms; (ii) a modified GSZ- Z_p^r variant employing an effective radius-dependent nuclear charge; and (iii) the binding energy screening (BES) approximation, which treats the projectile as a rigid Coulomb core. For the bare ion (C^{6+}), the captured electron’s final state is described by a hydrogenic wavefunction [26], while, for partially dressed ions ($q = 1\text{--}5$), Slater-type orbitals are employed [27]. Given the importance of carbon ions in radiotherapy applications, we use the computed cross-sections to evaluate the average binding energy for the different carbon ions, which is generally approximated by the projectile ionization energies (IEs) [12], a key quantity in stopping power calculations.

Unless otherwise stated, atomic units (a.u.) are used throughout this work.

2. Theory

We treat the atomic collision as a system comprising a projectile and a multielectron target with nuclear charge Z_T . The projectile electrons and the passive (non-active) target electrons are assumed to remain frozen in their initial states during the collision; i.e., we adopt the frozen core approximation. The projectile, with nuclear charge Z_p , is partially screened by its bound electrons, resulting in a net ionic charge $q = Z_p - N_p$, where N_p is the number of bound electrons. We employ the independent electron model (IEM)

together with the straight-line impact-parameter approximation, for which the internuclear separation is given by

$$\mathbf{R} = \mathbf{b} + \mathbf{v}t, \quad (1)$$

where $\mathbf{R}$ is the internuclear vector, $\mathbf{b}$ the impact parameter (perpendicular to the relative velocity), $\mathbf{v}$ the constant collision velocity, and t the time. Following the method proposed by Martínez et al. [28], where the multielectron problem is reduced to a one-active-electron description, the resulting Hamiltonian for the active electron reads

$$H = -\frac{1}{2}\nabla^2 + V_T(\mathbf{x}) + V_P(\mathbf{s}) + V_S(\mathbf{R}), \quad (2)$$

where $\mathbf{x}$ and $\mathbf{s}$ denote the position vectors of the active electron relative to the target and projectile nuclei, respectively. The potential $V_T(\mathbf{x})$ represents the interaction of the active electron with the target nucleus and its passive electrons. Based on the formalism of Refs. [25,28], the target potential can be expressed as

$$V_T(\mathbf{x}) = -\frac{Z_T}{x} + \sum_{i=1}^M \left\langle \phi_i(\mathbf{x}_{Ti}) \left| \frac{1}{|\mathbf{x} - \mathbf{x}_{Ti}|} \right| \phi_i(\mathbf{x}_{Ti}) \right\rangle. \quad (3)$$

where $\phi_i(\mathbf{x}_{Ti})$ is the initial-state wavefunction of the i -th passive target electron, and $\mathbf{x}_{Ti}$ is its position relative to the target nucleus. $V_P(\mathbf{s})$ describes the interaction between the active electron and the projectile. $V_S(\mathbf{R})$ accounts for four Coulomb interactions: (i) between the projectile and target nuclei; (ii) between the projectile electrons and the target passive ones; (iii) between the target nucleus and the projectile electrons; and (iv) between the projectile nucleus and the target passive electrons, yielding

$$\begin{aligned} V_S(\mathbf{R}) = & \frac{Z_P Z_T}{R} + \sum_{i=1}^M \sum_{j=1}^N \left\langle \phi_i(\mathbf{x}_{Ti}) \phi_j(\mathbf{s}_{Pj}) \left| \frac{1}{|\mathbf{x}_{Ti} - \mathbf{R} - \mathbf{s}_{Pj}|} \right| \phi_i(\mathbf{x}_{Ti}) \phi_j(\mathbf{s}_{Pj}) \right\rangle \\ & - \sum_{j=1}^N \left\langle \phi_i(\mathbf{s}_{Pj}) \left| \frac{Z_T}{|\mathbf{R} + \mathbf{s}_{Pj}|} \right| \phi_i(\mathbf{s}_{Pj}) \right\rangle - \sum_{i=1}^M \left\langle \phi_i(\mathbf{x}_{Ti}) \left| \frac{Z_P}{|\mathbf{R} - \mathbf{x}_{Ti}|} \right| \phi_i(\mathbf{x}_{Ti}) \right\rangle. \end{aligned} \quad (4)$$

Here, $\phi_j(\mathbf{s}_{Pj})$ denotes the initial wavefunction of the j -th bound projectile electron, with $\mathbf{s}_{Pj}$ representing its position relative to the projectile nucleus.

As a given $V_S(\mathbf{R})$ depends only on the internuclear distance, it contributes a pure phase factor to the scattering amplitude. As shown in Ref. [29], this phase affects only differential cross-sections that depend on the projectile scattering angle and does not influence the total capture cross-section [25]. The first-order prior-form transition amplitude as a function of impact parameter $\mathbf{b}$ is thus

$$\mathcal{A}_{if}^-(\mathbf{b}) = a_{if}^-(\mathbf{b}) \exp \left[-i \int_{-\infty}^{\infty} V_S(\mathbf{R}) dt \right], \quad (5)$$

where $a_{if}^-(\mathbf{b})$ is the reduced amplitude that governs the total cross-section. Then, on computing a_{if} , the $V_S(\mathbf{R})$ term may be omitted from the electronic Hamiltonian $H_e = H - V_S(\mathbf{R})$, yielding

$$a_{if}^-(\mathbf{b}) = -i \int_{-\infty}^{\infty} dt \left\langle \chi_f^- \left| \left(H_e - i \frac{\partial}{\partial t} \right) \right| \chi_i^+ \right\rangle. \quad (6)$$

The distorted initial and final channel wavefunctions are given by

$$\chi_i^+(\mathbf{x}, \mathbf{s}, t) = \phi_i^{n_i l_i m_i}(\mathbf{x}) \exp(-i\epsilon_i t) \mathcal{L}_i^+(\mathbf{s}), \quad (7)$$

$$\chi_f^-(\mathbf{x}, \mathbf{s}, t) = \phi_f^{n_f l_f m_f}(\mathbf{s}) \exp\left(-i\frac{1}{2}v^2 t + i\mathbf{v} \cdot \mathbf{x} - i\epsilon_f t\right) \mathcal{L}_f^-(\mathbf{x}), \quad (8)$$

where $\phi_i^{n_i l_i m_i}(\mathbf{x})$ and $\phi_f^{n_f l_f m_f}$ are the initial and final bound-state wavefunctions (characterized by quantum numbers $n_i l_i m_i$, and $n_f l_f m_f$, respectively). $\mathcal{L}_i^+$, $\mathcal{L}_f^-$ are distortion factors accounting for continuum interactions in the entrance channel between the projectile and the active electron and in the exit channel between the target and the active electron, respectively. These wavefunctions satisfy the time-dependent Schrödinger equation in the respective entrance and exit channels [25].

As stated above, the projectile potential $V_P(\mathbf{s})$ accounts for the interaction between the active electron and the bound electrons of the projectile and can be written as

$$V_P(\mathbf{s}) = -\frac{Z_P}{s} + \sum_{j=1}^N \left\langle \varphi_i(\mathbf{s}_{Pj}) \left| \frac{1}{|\mathbf{s} - \mathbf{s}_{Pj}|} \right| \varphi_i(\mathbf{s}_{Pj}) \right\rangle. \quad (9)$$

In practice, this potential is modeled using two distinct approaches. The first approach follows the model proposed in [25], which employs the two-parameter analytical Green–Sellin–Zachor (GSZ) potential [30], where the projectile potential is expressed as the sum of a long-range Coulomb term and a short-range screening contribution

$$V_P(s) = -\frac{q}{s} - \frac{(Z_P - q)}{s} \Omega(s), \quad (10)$$

with

$$\Omega(s) = [H(\exp(s/d) - 1) + 1]^{-1}, \quad (11)$$

which describes the screening due to the projectile's bound electrons. The parameters H and d depend on the projectile's nuclear charge Z_P and its net charge state q . Their values are reported in Table 1 [30,31].

Table 1. Parameters H and d for C^{q+} projectiles [30].

Projectile	H (a.u.)	d (a.u.)
C^+	2.000	0.939
C^{2+}	1.520	0.613
C^{3+}	1.065	0.360
C^{4+}	0.716	0.190
C^{5+}	0.570	0.100

In the second approach, the projectile ion is treated as a rigid core, with an effective charge Z_P determined via the binding energy screening (BES) approximation proposed by Das et al. [32], which accounts for the screening effect of the bound electrons. The screened nuclear charge is defined as

$$\tilde{Z}_P = \sqrt{-2n_f^2 \epsilon_f}, \quad (12)$$

where n_f and ϵ_f are the principal quantum number and the binding energy of the final captured state, respectively. The values of ϵ_f are reported in Table 2 [33]. The corresponding projectile potential is then

$$V_P(s) = -\frac{\tilde{Z}_P}{s}. \quad (13)$$

Table 2. Values of ϵ_f (a.u.) for each final excited state of C^{q-1} ions.

C^0	ϵ_f	C^+	ϵ_f	C^{2+}	ϵ_f
—	—	—	—	$1s^22s^2$	−1.6831
$1s^22s^22p^2$	−0.3962	$1s^22s^22p^1$	−0.8836	$1s^22s^12p^1$	−1.2361
$1s^22s^22p^13s^1$	−0.1301	$1s^22s^23s^1$	−0.3605	$1s^22s^13s^1$	−0.6553
$1s^22s^22p^13p^1$	−0.0947	$1s^22s^23p^1$	−0.2843	$1s^22s^13p^1$	−0.5469
$1s^22s^22p^13d^1$	−0.0548	$1s^22s^23d^1$	−0.2284	$1s^22s^13d^1$	−0.4963
$1s^22s^22p^14s^1$	−0.0563	$1s^22s^24s^1$	−0.1759	$1s^22s^14s^1$	−0.3374
$1s^22s^22p^14p^1$	−0.0448	$1s^22s^24p^1$	−0.1417	$1s^22s^14p^1$	−0.3009
$1s^22s^22p^14d^1$	−0.0305	$1s^22s^24d^1$	−0.1281	$1s^22s^14d^1$	−0.2802
$1s^22s^22p^15s^1$	−0.0315	$1s^22s^25s^1$	−0.1043	$1s^22s^15s^1$	−0.2070
$1s^22s^22p^15p^1$	−0.0218	$1s^22s^25p^1$	−0.0913	$1s^22s^15p^1$	−0.1900
$1s^22s^22p^15d^1$	−0.0199	$1s^22s^25d^1$	−0.0817	$1s^22s^15d^1$	−0.1796
C^{3+}	ϵ_f	C^{4+}	ϵ_f		
—	—	$1s^2$	−14.370		
$1s^22s^1$	−2.3658	$1s^12s^1$	−3.4016		
$1s^22p^1$	−2.0689	$1s^12p^1$	−3.0963		
$1s^23s^1$	−0.9891	$1s^13s^1$	−1.4629		
$1s^23p^1$	−0.9098	$1s^13p^1$	−1.3876		
$1s^23d^1$	−0.8893	$1s^13d^1$	−1.3972		
$1s^24s^1$	−0.5410	$1s^14s^1$	−0.8157		
$1s^24p^1$	−0.5089	$1s^14p^1$	−0.7859		
$1s^24d^1$	−0.5002	$1s^14d^1$	−0.7897		
$1s^25s^1$	−0.3406	$1s^15s^1$	−0.5214		
$1s^25p^1$	−0.3245	$1s^15p^1$	−0.5066		
$1s^25d^1$	−0.3201	$1s^15d^1$	−0.5085		

When potential $V_p(s)$ is described by the GSZ approach, see (10), the scattering amplitude decomposes into two distinct contributions: one arising from the long-range Coulomb term and the other from the short-range screening part of the potential. Using (6), the reduced transition amplitude can be expressed as

$$a_{if}^-(\mathbf{b}) = a_{if}^{-(a)}(\mathbf{b}) + a_{if}^{-(s)}(\mathbf{b}), \quad (14)$$

where $a_{if}^{-(a)}(\mathbf{b})$ corresponds to the long-range Coulomb contribution, and $a_{if}^{-(s)}(\mathbf{b})$ represents the short-range contribution. Conversely, in the rigid core approximation (BES model (13)) or for bare projectiles, the short-range term does not exist, i.e., $a_{if}^{-(s)}(\mathbf{b}) = 0$, since the interaction is purely Coulombic, and only the long-range component contributes to the transition amplitude. Within the CDW-EIS framework, the initial- and final-channel distortion functions are defined as

$$\mathcal{L}_i^+(s) = \exp[-i\nu \ln(vs + \mathbf{v} \cdot \mathbf{s})] \quad (15)$$

$$\mathcal{L}_f^-(x) = N^*(\zeta) {}_1F_1[-i\zeta; 1; -i(vx + \mathbf{v} \cdot \mathbf{x})] \quad (16)$$

where v is the projectile velocity, with $\nu = q/v$ and $\zeta = \tilde{Z}_T/v$. The normalization factor of the confluent hypergeometric function ${}_1F_1$ is given by $N(a) = \exp(\pi a/2)\Gamma(1 - ia)$, with Γ denoting the Euler gamma function. The effective target charge $\tilde{Z}_T$ is determined according to Belkić's criterion $\tilde{Z}_T = \sqrt{-2n_i^2\epsilon_i}$, where n_i and ϵ_i are the principal quantum number and binding energy of the initial target orbital, respectively.

The initial and final bound states, $\phi_i^{n_i l_i m_i}(\mathbf{x})$ and $\phi_f^{n_f l_f m_f}(\mathbf{s})$, are expressed as linear combinations of Slater-type orbitals (STOs):

$$\phi(\mathbf{r}) = \sum_k C_k S_{n_k, l_k, m_k}(\mathbf{r}), \quad (17)$$

where $\phi(\mathbf{r})$ denotes either the initial or final bound-state wavefunction. The Slater-type orbitals are defined as

$$S_{n_k, l_k, m_k}(\mathbf{r}) = N_{n_k} r^{n_k-1} \exp(-Z_k r) Y_{l_k}^{m_k}(\hat{\mathbf{r}}), \quad (18)$$

with normalization constant

$$N_{n_k} = (2Z_k)^{(n_k+1/2)} [(2n_k)!]^{-1/2}. \quad (19)$$

Here, $Y_l^m(\hat{\mathbf{r}})$ are the normalized complex spherical harmonics, and Z_k is an effective orbital exponent. The expansion coefficients C_k , exponents Z_k , and quantum numbers n_k, l_k (with $m_k = -l_k, \dots, l_k$) for various atoms are tabulated in [34]. For final excited states of carbon ions, these parameters are taken from [27,33]. In the case of a bare projectile (e.g., C^{6+}), the final state is described by a hydrogenic wavefunction, as detailed in [26]. By applying a Fourier transform to the impact-parameter-dependent amplitude $a_{if}^-(\mathbf{b})$ in (14), one obtains the transition amplitude in momentum space:

$$\mathcal{R}_{if}^-(\boldsymbol{\eta}) = \int d\mathbf{b} \exp(i\mathbf{b} \cdot \boldsymbol{\eta}) a_{if}^-(\mathbf{b}), \quad (20)$$

where $\boldsymbol{\eta}$ denotes the transverse momentum transfer. This formulation enables an analytical evaluation of the cross-sections [35]. The differential capture cross-section for a transition from an initial state $(n_i l_i m_i)$ to a final state $(n_f l_f m_f)$, as a function of the projectile velocity v , is then given by

$$\sigma_{if}(v) = \int d\boldsymbol{\eta} |\mathcal{R}_{if}^-(\boldsymbol{\eta})|^2. \quad (21)$$

2.1. Details of Projectile Potential Model

The choice of the projectile potential model is crucial, particularly as the projectile charge state decreases, because bound projectile electrons significantly screen its nuclear charge at low q . For instance, for a C^+ projectile, notable discrepancies arise between the potentials generated by the BES and GSZ approaches. Specifically, in the GSZ approach, the short-range part is scaled by $(Z_P - q = 5)$, which may lead to an overestimation of the potential. To address this limitation and ensure physical consistency, we implement a thorough calculation of the effective charge based on the projectile electron density ρ . This effective charge, denoted Z_P^r replaces the nuclear charge Z_P in the scaling term of the GSZ short-range potential. The modified GSZ potential also satisfies the correct asymptotic limit, $sV(s) = q$ as $s \rightarrow \infty$, given by

$$V_P(s) = -\frac{q}{s} - \frac{(Z_P^r - q)}{s} \Omega(s). \quad (22)$$

The spherically averaged electron density ρ is obtained from the Slater-type orbital expansions of the projectile [27,33]. Thus, Z_P^r , the effective charge at radius r , is defined via Gauss's law as

$$Z_P^r = Z_P - \int_0^r 4\pi r'^2 \rho(r') dr'. \quad (23)$$

This expression represents the net positive charge of a test particle at distance r , accounting for screening by all electrons interior to that radius. To characterize the effective charge experienced by an electron in a given atomic orbital nl , we evaluate Z_p^r at the orbital root mean square (RMS) radius,

$$r = r_{\text{RMS}}^{(nl)} = \sqrt{\langle r^2 \rangle_{nl}} = \left[\int_0^\infty 4\pi r'^4 \rho_{nl}(r') dr' \right]^{1/2}, \quad (24)$$

where $\rho_{nl}(r')$ is the spherically averaged density contribution from orbital nl . The RMS radius provides a physically meaningful measure of the orbital's spatial extent that weights contributions by r'^2 , making it more sensitive to the diffuse tail of the wavefunction than the mean radius $\langle r \rangle_{nl}$. Finally, we compute the effective charge Z_p^r for each orbital of interest. These values, reported in Table 3, are used to parameterize the GSZ potential employed in the present calculations. We note that the values of the effective charge Z_p^r are close to those computed with the BES approach (12).

Table 3. Parameters Z_p^r and r for C^{q+} projectiles.

Projectile	Orbital	r (a.u.)	Z_p^r	$\tilde{Z}_p$ BES (12)
C^+	$1s^2 2s^2 2p^1$	1.5892	2.04	1.78
C^{2+}	$1s^2 2s^2$	1.4476	2.74	2.65
C^{3+}	$1s^2 2s^1$	1.3682	3.38	3.67
C^{4+}	$1s^2$	0.3115	4.64	4.35
C^{5+}	$1s^1$	0.2887	5.32	5.36

2.2. Water Molecule Description

The ground-state molecular orbitals are represented as linear combinations of atomic orbitals (LCAO). The corresponding binding energies are obtained using the molecular orbital–linear combination of atomic orbital self-consistent field (MO-LCAO-SCF) method, while the complete neglect of differential overlap (CNDO) approximation was employed to analyze the effective electron occupation of the various molecular orbitals [36]. The effective atomic electron populations and orbital binding energies for the water molecule, as reported by Siegbahn et al. [36], are summarized in Table 4.

Table 4. Electron populations and binding energies for water.

Molecular Orbital	Population	Binding Energy ϵ_l (a.u.)
1a ₁	2.0 O _{1s}	−19.84
2a ₁	1.48 O _{2s} + 0.52 H _{1s}	−1.18
1b ₂	1.18 O _{2p} + 0.82 H _{1s}	−0.67
3a ₁	0.22 O _{2s} + 1.44 O _{2p} + 0.34 H _{1s}	−0.54
1b ₁	2.0 O _{2p}	−0.46

Accordingly, the electron capture cross-section from a given molecular orbital l to a final state f is expressed as

$$\sigma_{lf} = \sum_{j=1}^{N_l} c_{lj} \sigma_{if,j}, \quad (25)$$

where N_l is the number of atomic centers contributing to molecular orbital l , $\sigma_{if,j}$ is the cross-section for electron capture from the j -th atomic orbital in the LCAO expansion, and c_{lj} represents the corresponding effective atomic electron population (i.e., the occupation-weighted coefficient) associated with that atomic center. The atomic orbitals are described

using Roothaan–Hartree–Fock wavefunctions from Ref. [34]. In the evaluation of Belkić’s effective target charge, $\tilde{Z}_T = \sqrt{-2n^2\epsilon_l}$, we use the molecular orbital energy ϵ_l listed in Table 4. Finally, the total electron capture cross-section is obtained by summing over all final states:

$$\sigma_{Tot} = \sum_f \sigma_{lf}. \quad (26)$$

3. Results and Discussions

3.1. Total Cross-Section

In this section, we present the total cross-sections for single-electron capture from water molecules by C^{q+} projectiles ($q = 1-6$) over the collision energy range from 40 keV/u to 10 MeV/u, computed within the prior form of the CDW-EIS approximation. Three distinct models are employed to describe the projectile–electron interaction potential: (i) the GSZ potential, which combines a long-range Coulomb term with a short-range screening contribution, (ii) the modified GSZ potential (GSZ- Z_p') (22), and (iii) the binding energy screening (BES) approximation, in which the projectile is treated as a rigid Coulomb core. As noted above, for bare projectiles (e.g., C^{6+}), the final captured state is described by a hydrogenic wavefunction [26]; we include all final states up to $n_f = 5$, $l_f = 4$, $m_f = -l_f, \dots, l_f$. For dressed projectiles (C^{q+} with $q = 1-5$), the final states are described by Slater-type orbitals, as reported by Novikov [27], which include excited states up to d -type symmetry ($n_f = 5$, $l_f = 2$, $m_f = -l_f, \dots, l_f$).

In Figure 1, we present the TCS for electron capture by carbon ions with charge states $q = 1-6$. Due to the lack of experimental data for water, the present theoretical results are compared with measurements reported by Anholt et al. [37] for H_2 and O_2 , scaled to H_2O using Bragg’s additivity rule. For the C^{3+} case, we include the measured cross-section for H^+ production from water fragmentation induced by electron capture [24]. As stated by the authors, H^+ is one of several target fragments (i.e., H_2O^+ , OH^+ , O^+ , O_2^+ , O_3^+ , and H^+) that arise from the capture process. Thus, this measured cross-section should be considered a lower bound on the total electron capture cross-section, since contributions from other fragmentation channels were not reported [24]. Additionally, for the C^{4+} case, experimental data for electron capture on water molecules reported by Maurya et al. [17] are included for comparison. At low charge states ($q = 1-2$), the GSZ potential systematically overestimates the TCS compared to BES, while the GSZ- Z_p' potential reproduces BES results closely. This behavior, anticipated in Section 2.1, arises because the standard GSZ form inadequately treats short-range screening when the number of bound electrons approaches the nuclear charge ($N \approx Z_p$), a limitation addressed by the effective charge Z_p' . As the charge state increases and projectile screening becomes less significant, the results from the three approximations converge. Also, a comparison with the CTMC calculations of Liamsuwan [12] is provided for all charge states. We note a large systematic discrepancy of approximately one order of magnitude between the present CDW-EIS predictions and the CTMC results across the entire energy range considered. However, for the C^+ case, the CDW-EIS results obtained with the BES and GSZ- Z_p' approaches converge toward the CTMC data as the collision energy increases. Additionally, for the C^{6+} case, we include CTMC results from Tran et al. [38] and Illescas et al. [39]. These are in good agreement with the present CDW-EIS calculations. In contrast, the CTMC results of Liamsuwan [12] appear to underestimate the cross-sections by at least an order of magnitude compared to other theoretical approaches.

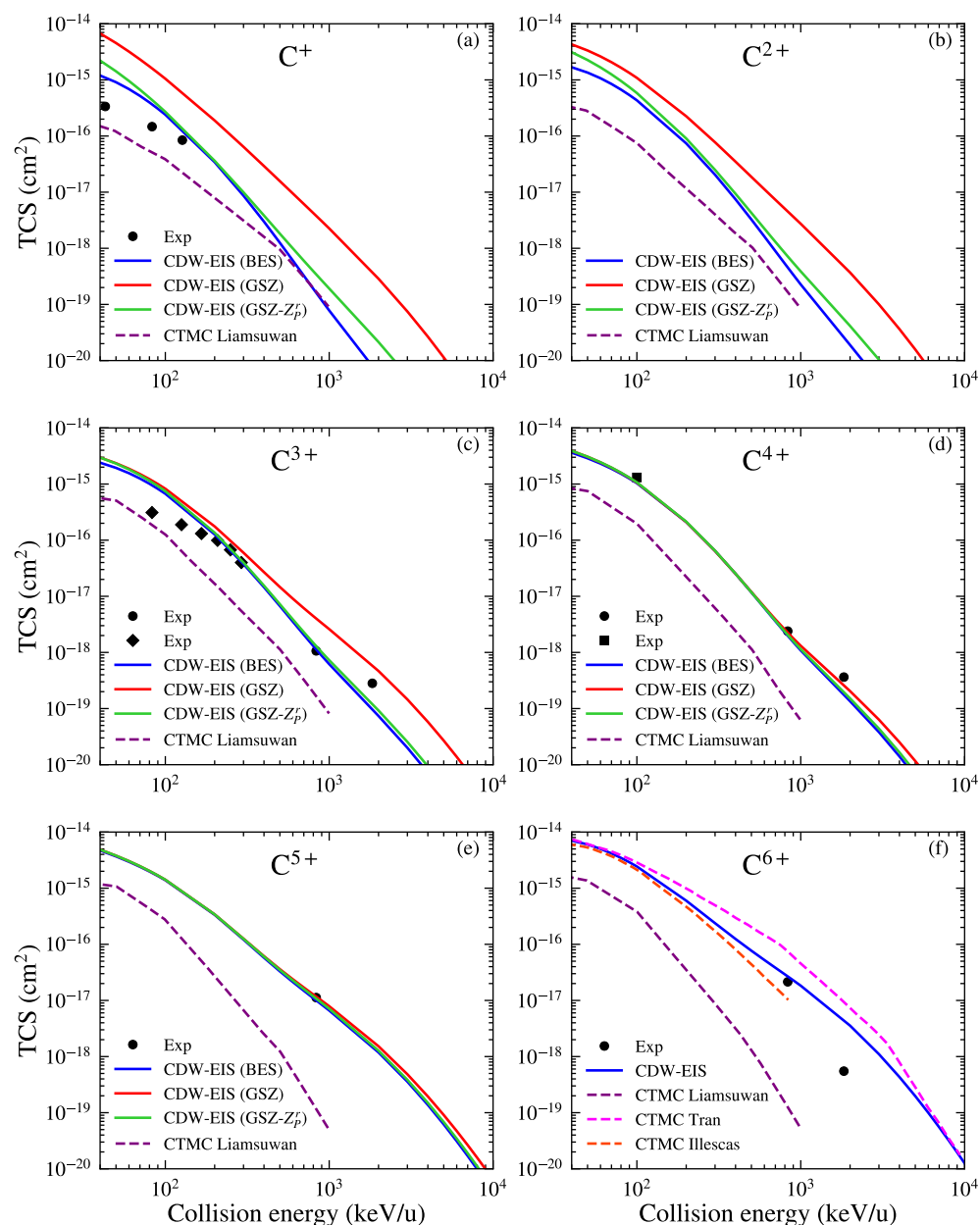


Figure 1. TCS for electron capture by (a) C^+ , (b) C^{2+} , (c) C^{3+} , (d) C^{4+} , (e) C^{5+} , and (f) C^{6+} from water molecules as function of impact energy. Present theoretical calculations (solid lines): CDW-EIS (BES) (blue), CDW-EIS (GSZ) (red) and CDW-EIS (GSZ- Z_p^r) (green). Others theories (dashed lines): CTMC Liamsuwan (purple) [12], CTMC (magenta) [38], and CTMC Illescas (orange) [39]. Experimental data from [37] (Bragg's rule) (circles), [24] (diamonds) and [17] (square).

Figure 2 shows the contributions of individual initial molecular orbitals to the total electron capture cross-section. We observe that the CDW-EIS results obtained with the GSZ- Z_p^r approach for all studied projectile charge states, C^{q+} ($q = 1-6$), exhibit similar general trends. At impact energies below a few hundred keV/u, the valence orbital $1b_1$ dominates over all other orbitals. Furthermore, the contribution of each orbital is approximately inversely proportional to its binding energy: more closely bound orbitals yield smaller cross-sections. In the high-energy regime (≥ 1 MeV/u), the innermost orbital $1a_1$ provides the dominant contribution to the TCS. As charge exchange requires momentum matching, the characteristic velocity of the captured electron must be comparable to the projectile velocity. At high impact energies, only the tightly bound $1a_1$ orbital possesses a sufficient mean linear momentum to satisfy this condition [40,41].

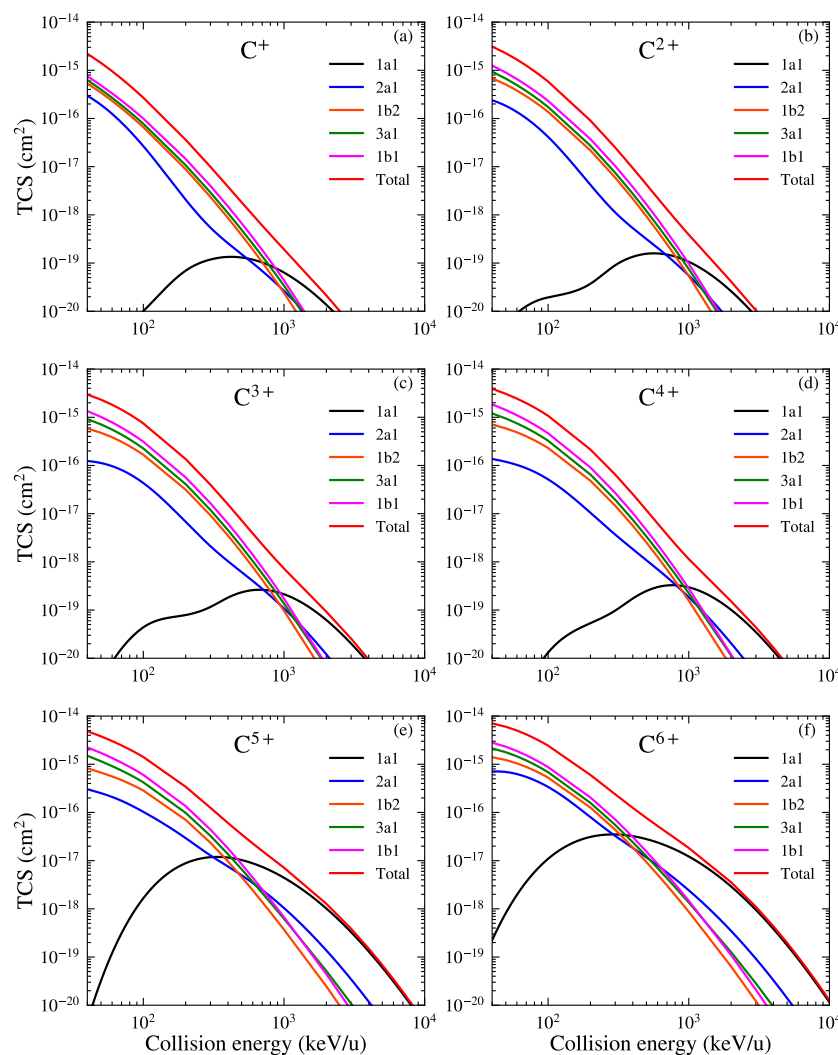


Figure 2. TCS for electron capture by (a) C^+ , (b) C^{2+} , (c) C^{3+} , (d) C^{4+} , (e) C^{5+} , and (f) C^{6+} from water molecules as function of impact energy. Present theoretical CDW-EIS calculations (GSZ- Z_p^p). Water molecule orbitals in solid lines: $1a_1$ (black), $2a_1$ (blue), $1b_2$ (orange), $3a_1$ (green), $1b_1$ (magenta) and total (red).

For completeness, Figure 3 presents an analysis of the contributions from final bound states to the TCS, computed using the CDW-EIS formalism with the GSZ- Z_p^p projectile potential. At collision energies below a few hundred keV/u and for projectile charge states $q = 1-3$, the final $n_f = 2$ state provides the dominant contribution to the TCS. Notably, for the C^+ projectile, the $n_f = 2$ final-state contribution and the total TCS curve are nearly indistinguishable (see Figure 3a). This behavior arises because the electron captured into the final C^0 state with configuration $(1s^2 2s^2 2p^2)$ has a binding energy $\epsilon_f = -0.396250$ a.u., which closely matches the energy of the $1b_1$ molecular orbital of water (Table 4), which is a signature of resonant electron capture. For C^{4+} (Figure 3d), the $n_f = 2$ and $n_f = 3$ contributions are comparable. As the charge increases to $q = 5-6$, the dominant contribution shifts to $n_f = 3$. Furthermore, for all projectiles at energies above ~ 1 MeV/u, lower n_f final states generally dominate, with contributions decreasing monotonically: $n_f = 2 > n_f = 3 > n_f = 4 > n_f = 5$. However, in the high-energy regime (≥ 1 MeV/u) for C^{5+} and C^{6+} projectiles, the innermost final state ($n_f = 1$) becomes the most significant contributor to the TCS. This can be understood by considering the time-reversed state-to-state reaction: at high impact velocities, the momentum distribution of the $n_f = 1$ projectile's state provides the best match to the projectile's linear momentum [41].

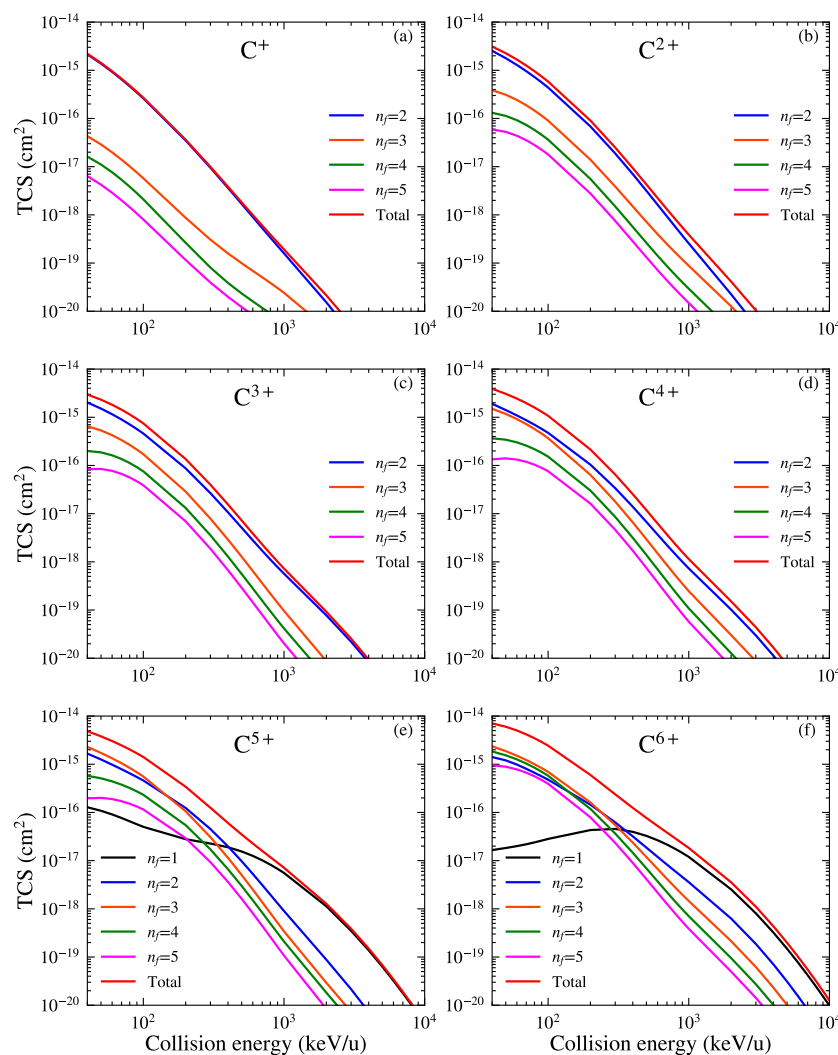


Figure 3. TCS for electron capture by (a) C^+ , (b) C^{2+} , (c) C^{3+} , (d) C^{4+} , (e) C^{5+} , and (f) C^{6+} from water molecules as function of impact energy. Present theoretical CDW-EIS calculations (GSZ- Z_p^r) (solid lines). Final selective state: $n_f = 1$ (black), $n_f = 2$ (blue), $n_f = 3$ (orange), $n_f = 4$ (green), $n_f = 5$ (magenta) and total (red).

3.2. Q-Charge Analysis

Figure 4a shows the TCS dependence on the projectile's charge state q . The CDW-EIS results with the GSZ- Z_p^r and BES approaches at 70, 200, and 400 keV/u follow the trends reported by Greenwood et al. [20] and Otranto et al. [11] at much lower energies (a few keV/u). In contrast, the standard GSZ potential deviates for low charge states ($q = 1-2$). For comparison, we include the nonlinear fit of Otranto et al. [11]:

$$\sigma_{fit} = 10^{-16} a q^b \quad (\text{in cm}^2), \quad (27)$$

where the parameters a and b are energy-dependent. Using the CDW-EIS model with GSZ- Z_p^r potential, we obtain the following results for the three collision energies considered:

$$\begin{aligned} 70 \text{ keV/u : } & a = 6.325, \quad b = 0.875; \\ 200 \text{ keV/u : } & a = 0.324, \quad b = 1.445; \\ 400 \text{ keV/u : } & a = 0.0294, \quad b = 1.703. \end{aligned}$$

In order to characterize the general trend of the TCS for different projectile charge states q as a function of collision energy, we examine—using CDW-EIS calculations with the

GSZ- Z_p^r and BES potential approaches—the ratio σ_q/σ_6 , as shown in Figure 4b. Here, σ_q denotes the TCS for a C^{q+} projectile, and σ_6 refers to that of the fully stripped C^{6+} ion. Across the energy range studied, the ratios computed with the two potential approaches agree well for highly charged projectiles ($q \geq 3$), where screening effects are minimal. In particular, for $q = 5$, the ratio is nearly constant over the full energy range. In contrast, for low charge states ($q = 1-2$), discrepancies emerge in the high-energy regime, reflecting differences in the treatment of short-range screening. Regarding the energy dependence, at higher energies, the ratios σ_q/σ_6 are comprehended in the range between 10^{-4} and 10^{-1} . At impact energies below a few hundred keV/u, the ratios σ_q/σ_6 lie in the range between 10^{-1} and 1. Consequently, for low impact-energies, a precise description of the electron capture process for each projectile charge state q is relevant. This is particularly important in radiobiological applications, e.g., hadrontherapy, where accurate modeling of Bragg's peak, i.e., the region where heavy particles give the highest contribution to dose deposition, is critical [42].

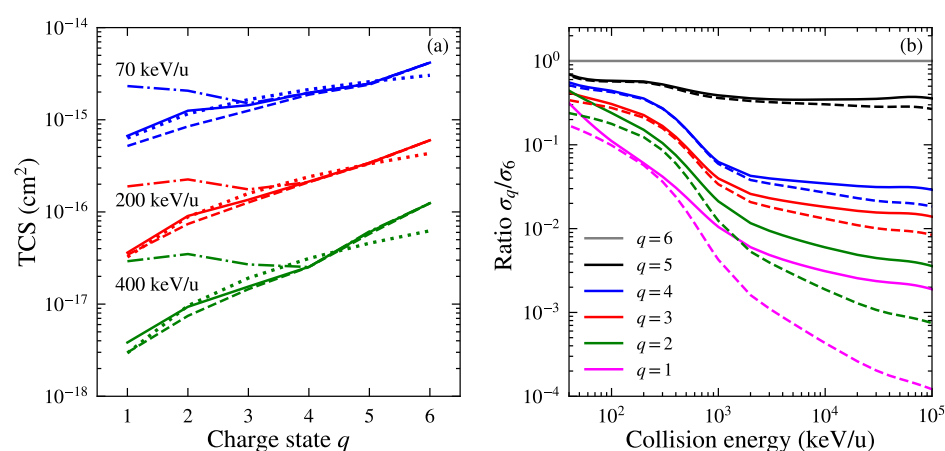


Figure 4. (a) TCS for electron capture by C^{q+} from water molecules as function of charge state q . Present theoretical calculations: CDW-EIS (GSZ- Z_p^r) (solid lines), CDW-EIS (BES) (dashed lines), CDW-EIS (GSZ) (dashdot lines), and nonlinear fit (dotted lines) for given collision energies of 70 keV/u (blue), 200 keV/u (red), and 400 keV/u (green). (b) TCS ratios σ_q/σ_6 as function of impact energy. Present theoretical calculations: CDW-EIS (GSZ- Z_p^r) (solid lines) and CDW-EIS (BES) (dashed lines).

3.3. Average Binding Energy

In stopping power calculations [12], the mean energy loss per single electron capture event is given by

$$\Delta E_c = \frac{T}{\lambda} + \langle B \rangle_{\text{H}_2\text{O}} - \langle B \rangle_{C^{(q-1)+}}, \quad (28)$$

where T/λ accounts for the kinetic energy required to accelerate the captured electron to the projectile's velocity. Here, T is the projectile energy per nucleon (in keV/u), and $\lambda \approx 1836$ is the proton-to-electron mass ratio. The term $\langle B \rangle_{\text{H}_2\text{O}}$ denotes the average binding energy of the electrons in the water molecule [12,43], while $\langle B \rangle_{C^{(q-1)+}}$ represents the average binding energy of the captured electron in the projectile ion after capture. This latter quantity is commonly approximated by the ionization energy (i.e., the first ionization potential) of the resulting $C^{(q-1)+}$ ion, as in previous stopping power calculations for He^{q+} and C^{q+} ions in water [12,43]. We compute the average binding energy $\langle B \rangle_{C^{(q-1)+}}$ by weighting the cross-section for electron capture (σ_f) into each final state (f) by its corresponding binding energy (ϵ_f ; see Table 2)

$$\langle B \rangle_{C^{(q-1)+}} = \frac{\sum_f \sigma_f \epsilon_f}{\sum_f \sigma_f}, \quad (29)$$

Following Equation (29), the average binding energy for a specific final principal quantum number n_f is obtained as

$$\langle B \rangle_{C^{(q-1)+}}^{n_f} = \frac{\sum_{l_f} \sigma_{n_f l_f} \epsilon_{n_f l_f}}{\sum_{l_f} \sigma_{n_f l_f}}, \quad (30)$$

where the sums run over all allowed orbital angular momentum states l_f for the given n_f .

In Figure 5, we report the computed average binding energies, obtained using Equations (29) and (30), and we compare them with the IE values reported in [12]. For comparison, we highlighted the region in the plot that corresponds to the full width at half maximum (FWHM) of the equilibrium charge-state fraction distribution from [12]. For C^{q+} projectiles with $q = 1-2$, the discrepancy in the outlined energy regions between the theoretical $\langle B \rangle_{C^{(q-1)+}}$ and the IE values is of the order of a few eV. In contrast, for higher charge states ($q = 4-6$), the discrepancy becomes significant, ranging from a few tens of eV up to a few hundred eV (e.g., for C^{5+}). As a result, the use of energy-independent IE values for higher charge states ($q = 4-6$) may not be adequate and could lead to an underestimation of the mean energy loss in stopping power calculations.

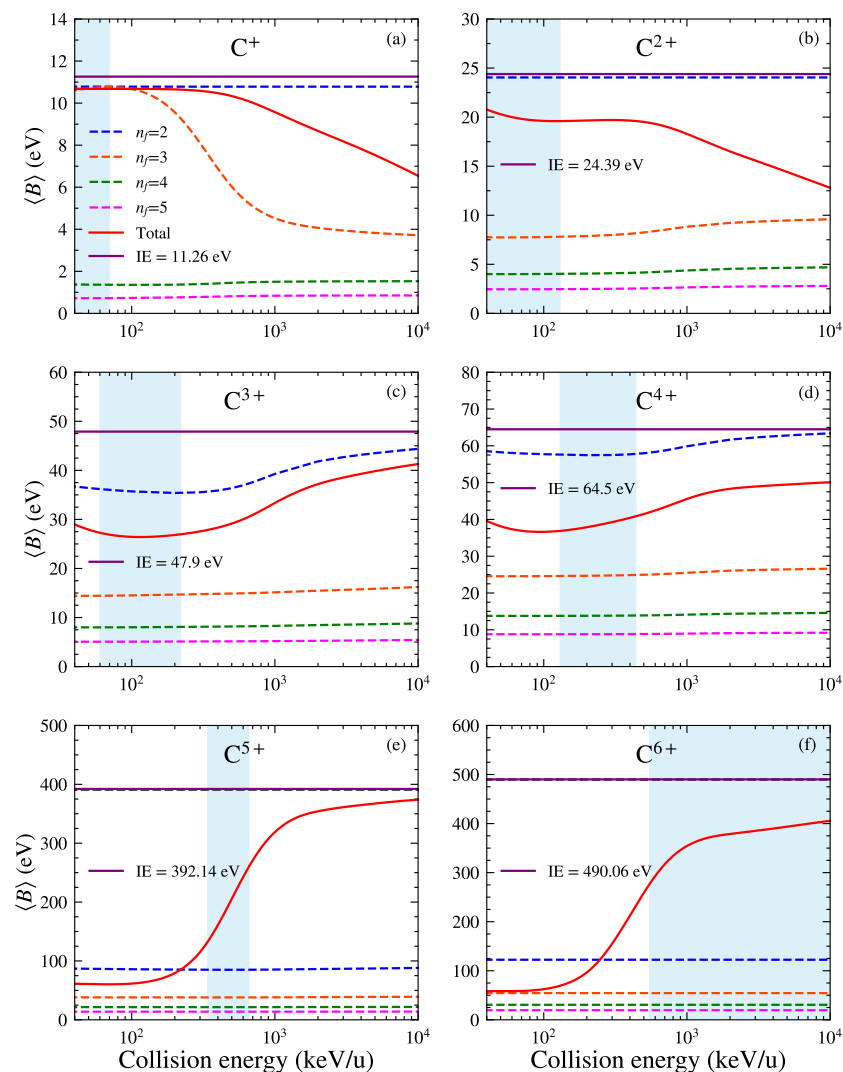


Figure 5. Average binding energy for (a) C^0 , (b) C^+ , (c) C^{2+} , (d) C^{3+} , (e) C^{4+} , and (f) C^{5+} ions as function of impact energy. Present theoretical CDW-EIS calculation (GSZ- Z_p^i). Final selective state: $n_f = 1$ (black), $n_f = 2$ (blue), $n_f = 3$ (orange), $n_f = 4$ (green), $n_f = 5$ (magenta) and total (red). The IE values (purple) from [12]. The shaded region represents the FWHM of the equilibrium charge-state fraction distribution from [12].

4. Conclusions

We presented the total cross-sections for single-electron capture in collisions of C^{q+} ($q = 1-6$) ions with water molecules over the energy range of 40 keV/u to 10 MeV/u, computed within the prior form of the CDW-EIS approximation. Three different descriptions of the projectile potential were employed: (i) the Green–Sellin–Zachor (GSZ) model, which includes both long-range Coulomb and short-range screening terms; (ii) the GSZ- Z_p' , a variant with an effective nuclear charge; and (iii) the binding energy screening (BES) approach, which treats the projectile as a rigid Coulomb core. For low charge states ($q = 1-2$), the GSZ predictions differ significantly from those of the GSZ- Z_p' and BES approaches. The GSZ potential overestimates the cross-sections, likely due to an inadequate representation of screening when the projectile retains many bound electrons. As the charge state increases, the three models converge, reflecting the diminishing role of projectile electron screening in highly stripped ions.

The analysis of initial- and final-state contributions reveals a clear energy-dependent hierarchy: at low energies ($\leq$ few hundred keV/u), electron capture from valence orbitals (e.g., $1b_1$ of H_2O) into final states with $n_f = 2$ dominates. This is particularly evident when the binding energies of the initial and final states closely match (a signature of resonant capture). In contrast, at higher energies, the dominant contribution to the cross-section originates from the inner-shell orbitals of the target, which primarily feed the $n_f = 1$ capture channel of the C^{5+} and C^{6+} projectiles in the MeV/u regime.

Comparison with available experimental data and CTMC calculations shows good agreement for C^{6+} , while discrepancies of up to an order of magnitude appear for lower charge states (highlighting the sensitivity of capture dynamics to the projectile's electronic structure).

The total electron capture cross-sections exhibit a dependence on the projectile charge state q . At low impact energies, the TCSs for carbon ions with charge states ($q = 1-5$) are comparable to those for fully stripped C^{6+} , with the σ_q/σ_6 ratios being of the same order of magnitude. However, at higher energies, the TCSs for C^{q+} ($q = 1-4$) become significantly smaller than those for C^{6+} , causing the σ_q/σ_6 ratio to decrease rapidly with increasing impact energy. As q increases, the cross-sections grow, reflecting the stronger Coulomb attraction of more highly charged projectiles. Finally, the variations in the charge exchange processes (namely, electron capture and loss [42]) are most pronounced in the energy range up to a few hundred keV/u, which corresponds to the Bragg peak region for carbon ions in biological tissue. An accurate description of electron capture in this regime is therefore fundamental for modeling charge state evolution and energy deposition in ion beam therapy applications.

Furthermore, our findings indicate that the conventional use of ionization energies becomes inadequate for higher projectile charge states ($q = 4-6$), potentially leading to a systematic underestimation of the mean energy loss. Incorporating average binding energies derived from final state-selective theoretical cross-sections is therefore essential for improving the accuracy of stopping power calculations in carbon ion therapy.

In future work, we intend to refine the description of the projectile–electron interaction by incorporating electron correlation effects within the bound states of the projectile. This approach is expected to provide a more precise representation of the short-range screening dynamics induced by projectile electrons. Additionally, we intend to extend the present study to other biologically relevant molecules (such as DNA bases and amino acids) to assess the role of molecular structure and composition in electron capture dynamics across a broader range of radiobiological targets.

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Abbreviations

The following abbreviations are used in this manuscript:

BES	Binding Energy Screening
CDW	Continuum Distorted Wave
CDW-EIS	Continuum Distorted Wave-Eikonal Initial State
CNDO	Complete Neglect of Differential Overlap
CTMC	Classical Trajectory Monte Carlo
DW	Distorted Wave
DNA	Deoxyribonucleic Acid
FWHM	Full Width at Half Maximum
GSZ	Green–Sellin–Zachor
IEM	Independent Electron Model
IE	Ionization Energy
LCAO	Linear Combinations of Atomic Orbitals
MO-LCAO-SCF	Molecular Orbital–Linear Combination of Atomic Orbital Self-Consistent Field
RMS	Root Mean Square
RNA	Ribonucleic Acid
TC-BGM	Two-Center Basis Generator Method
TCS	Total cross-section

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