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Partial Stopping Power Effective Charges (PSPEC) for Proton Beams in DNA and Liquid Water Using (MELF-GOS) Method for Valence and Inner Shells

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***Abstract* - The stopping of energetic ions in condensed matter is a complicated problem and represents a continuous challenge for both theoretical and experimental physicists. Even in the case of an idealized electron gas model for the target the problem is of many-body nature. In present work, the effects of outer and total subshell of partial stopping power effective charge (PSPEC) in DNA and liquid water has been studied using MELF-GOS model taking into consideration charge exchange (q) and electronic excitation in the target. Bragg's rule has been applied to get the stopping power of DNA and liquid water and the mathematical equations has been program by writing a Fortran-90 program for numerical calculations.**

***Keywords* - Stopping power, Effective charges, Bragg's rule, DNA, Liquid water, MELF-GOS, Valance shell, Inner shell.**

I. INTRODUCTION

Give accurate information about stopping power and energy loss of fast particles in matter is very important in many practical applications in many research areas for example microelectronics, surface analysis, nuclear physics, space exploration, protection against radiation, and radio-therapeutic medicine [1-6]. The dielectric formulation is one of the most promised techniques to describe the interaction of swift ions and other charged particles with matter [7]. There is a lot of experimental data in the previous work about the inelastic energy loss of fast projectiles in solids for different projectile target combinations [8], and several models have been developed to explain and predict these experimental results [9-13]. In present work, the Mermin-Energy-Loss-Function–Generalized-Oscillator Strength (MELF–GOS) method [13,14] applied to describe the energy-loss function of DNA and liquid water which calculated in the previous work [15], since it has been successfully used to describe the ELF of materials with a complex electronic spectrum [16-18]. Here the target electron excitations are split into two parts, one indicates to excitations of the inner-shell electrons, and the other produce from excitations of the outer (weakly bound) electrons, namely

$$\mathrm{Im}\left[\frac{-1}{\epsilon(\mathrm{k},\omega)}\right] = \mathrm{Im}\left[\frac{-1}{\epsilon(\mathrm{k},\omega)}\right]_{\mathrm{outer}} + \mathrm{Im}\left[\frac{-1}{\epsilon(\mathrm{k},\omega)}\right]_{\mathrm{inter}} \quad (1)$$

The excitations of the outer electrons of the solid, including both collective and single-particle excitations, are described by Mermin-type ELF,

$$\mathrm{Im}\left[\frac{-1}{\epsilon(\mathrm{k},\omega)}\right]_{\mathrm{outer}} = \mathrm{Im}\left[\frac{-1}{\epsilon(\mathrm{k}=0,\omega)}\right]_{\mathrm{exp}}$$
$$= \sum_i A_i \,\mathrm{Im}\left[\frac{-1}{\epsilon_m(\omega_i,\gamma_i,k=0,\omega)}\right]\Theta(\omega-\omega_{th,i}) \quad (2)$$

Where, $\in_M$ is the Mermin dielectric function [19]. The suitable parameter A_i and γ_i are represented position and width, respectively, of the ith Mermin-type ELF, while the coefficients A_i are the corresponding weights while $\hbar\omega_{th,i}$ is the threshold energy [20]. MELF-GOS model, in which the outer electron excitations of the target are accounted by Mermin-type energy loss functions, whereas the inner-shell electron excitations are modeled by the generalized oscillator strengths of the constituent atoms.

$$\mathrm{Im}\left[\frac{-1}{\epsilon(k,\omega)}\right]_{inner} = \frac{2\pi^2 N}{\omega}\sum_{nl}\frac{df_{nl}(k,\omega)}{d\omega} \quad (3)$$

Where, $df_{nl}(k,\omega)$ is the GOS of the (n,l) sub-shell and N is the molecular density of the target. In the present work the hydrogenic approach is used to get the GOS because it is analytical and describes the contribution of the K-shell ionization corresponding to C, N, O and P atoms well [13].

II. THEORETICAL BACKGROUND

Partial stopping power effective charge (PSPEC) of H-ions in DNA and liquid water

The Bragg additivity rule states that the stopping power of a medium is the sum of the stopping powers of its atomic components and is independent of both the chemical relationships between its constituents and the physical state of the medium [21].

$$S^{AB} = C_A S^A + C_B S^B \quad (4)$$

Where, C_A And $C_B = 1 - C_A$ are the molar fractions of component A and B, respectively.
Bragg's rule could be used to combine the stopping power of the compound and those of the constituent elements of the compound.
Bragg's rule expressed as follows:

$$(S)_{comp.} = \sum_i w_i s_i \quad (5)$$

Where, (s_i) is the stopping power of the element (i) in the composite, and

$$w_i = n_i A_i / A_c \quad (6)$$

Where, (w_i) is represents the percentage of presence of the element (i) in the composite (fraction by weight), (A_c, A_i) are the mass number of the composite and element (i) respectively,
Where:

$$A_c = \sum_i n_i A_i \quad (7)$$

and can be obtained on the amounts $(L_1, L_2, {}^{C}/_{Z_2})$ in terms of the mass stopping power of the equation:

$$f_{bragg's} = \frac{\sum_i W_i \langle Z/A \rangle_i f_i}{\langle Z/A \rangle_{comp.}} \quad (8)$$

Where, (f_i) is the amount of each of the five ingredients listed above.

$\langle {}^{Z}/_{A} \rangle_i$: The ratio between the average atomic number and mass number compound.

$$\langle Z/A \rangle_{comp.} = \sum_i w_i \left(\frac{Z}{A}\right)_i \quad (9)$$

The DNA-compound $C_{20}H_{27}N_7O_{13}P_2$ consists of 5-elements as shown and liquid water H_2O consists of two-elements, thus Brandt and Kitagawa have derived a formula for the (PSPEC) in a variational statistical approximation [22]; the stopping power of a singly charged projectile with velocity $\boldsymbol{v}$ can be expressed by:

$$S(q) \equiv \frac{dE}{dx} = \frac{2}{N\pi v^2} \int_0^\infty \frac{dk}{k} |\rho(k)|^2 \int_0^{kv} d\omega \omega Im \left[\frac{-1}{\epsilon(k,\omega)}\right] \quad (10)$$

Where, $\rho_q(k)$ is the Fourier transform of the projectile charge density given by [23]:

$$\rho(k) = z_1 \frac{q + (k\Lambda)^2}{1 + (k\Lambda)^2} \quad (11)$$

(Λ) represent the screening length [22].

By using the Eq. (10), one can calculates the stopping power $S(q)$ of each element in compounds, then apply Bragg's rule, for DNA:

$$S_{DNA}(q) = 20 S_C(q) + 27 S_H(q) + 7 S_N(q) + 13\, S_O(q) + 2 S_P(q) \quad (12)$$

For liquid water:

$$S_{H2O}(q) = 2 S_H(q) + S_O(q) \quad (13)$$

Eqs. (12, 13) apply for valance electrons. Taking the total subshell in the consideration by substitute Eq. (1) for energy loss fraction into Eq. (10),

$$S_{(q)} = \frac{2}{N\pi v^2} \int_0^\infty \frac{dk}{k} |\rho(k)|^2 \int_0^{kv} d\omega \omega \left[\mathrm{Im}\left[\frac{-1}{\epsilon(k,\omega)}\right]_{\text{outer}} + \mathrm{Im}\left[\frac{-1}{\epsilon(k,\omega)}\right]_{\text{total subshell}} \right] \quad (14)$$

The first term represents the stopping power of valance electrons as given in Eqs. (12, 13) and the second term represents the stopping power for total subshells, in other word:

$$S(q) = S_{outer}(q) + S_{total\ subshell}(q) \qquad (15)$$

To get the partial stopping power effective charge (PSPEC) ζ where $|\rho(k)| \to 1$ when $q \to 1$, therefore, is defined by [22]:

$$\zeta = \left[\frac{S_q}{S_{q=1}}\right]^{1/2} \qquad (16)$$

$$\left.\begin{aligned} \zeta_{outer}(q) &= \frac{S_{outer}(q)}{S_{outer}(q=1)} \\ \zeta_{total\ subshell}(q) &= \frac{S_{subshell}(q)}{S_{subshell}(q=1)} \end{aligned}\right\} \qquad (17)$$

III. RESULTS AND DISCUSSION

The following table illustrates the change in the value of partial stopping power effective charge (PSPEC) $\zeta(q)$ in figures (1-5) for outer and inner shell of DNA and liquid water at (q = 0) and (q = 1).

Figures (1-5) show the stopping parameter $\zeta(q)$ with ionization fraction (q) for different incident proton energy$T(0.05\ ,0.25, 1, 2, 2.5\ MeV/u)$ on DNA and liquid water at outer shell and subshell using (MELF-GOS) model. When $q \to 0$ $\zeta(q)$strongly dependent on incident proton energy in DNA and liquid water, while at $q \to 1, \zeta(q) \to 1$at different incident proton energy for both DNA and liquid water. There is minor difference between $\zeta(q)$ at outer shell and subshell at $q \to 0$, while they are exactly matched at $q \to 1$ as shown in table I.

Table I

Partial stopping power effective charge **ζ**(q) for outer and inner shell of DNA and liquid water at (q =0) and (q=1).

Charge fraction	Incident proton energy T (Mev /u)	ζ(q)			
		DNA		H_2O	
		Outer shell	Subshell	Outer shell	Subshell
q = 0	*0.05*	*0.16*	*0.08*	*0.16*	*0.025*
	0.25	*0.31*	*0.08*	*0.31*	*0.025*
	1	*0.41*	*0.08*	*0.41*	*0.025*
	2	*0.45*	*0.08*	*0.425*	*0.025*
	2.5	*0.46*	*0.08*	*0.45*	*0.025*
q = 1	*All value of energy*	$\zeta(q) = 1$			

IV.CONCLUSIONS

In the present work the excitation spectrum of the DNA and liquid water target has been described accurately by means of the MELF-GOS method [6, 7], which uses Mermin-type energy-loss functions for the outer electron excitations and generalized oscillator strengths for the inner-shell excitations. When$q \to 0$,$\zeta(q)$strongly dependent on incident proton energy in DNA and liquid water, while at $q \to 1, \zeta(q) \to 1$at different incident proton energy for both DNA and liquid water. There is minor difference between $\zeta(q)$ at outer shell and subshell at $q \to 0$, while they are exactly matched at $q \to 1$. The values of (ζ) have a significant dependence on velocity at low charge state $(\mathrm{q} = 0)$ while the dependence become less important at high charge state $(\mathrm{q} > 0)$.

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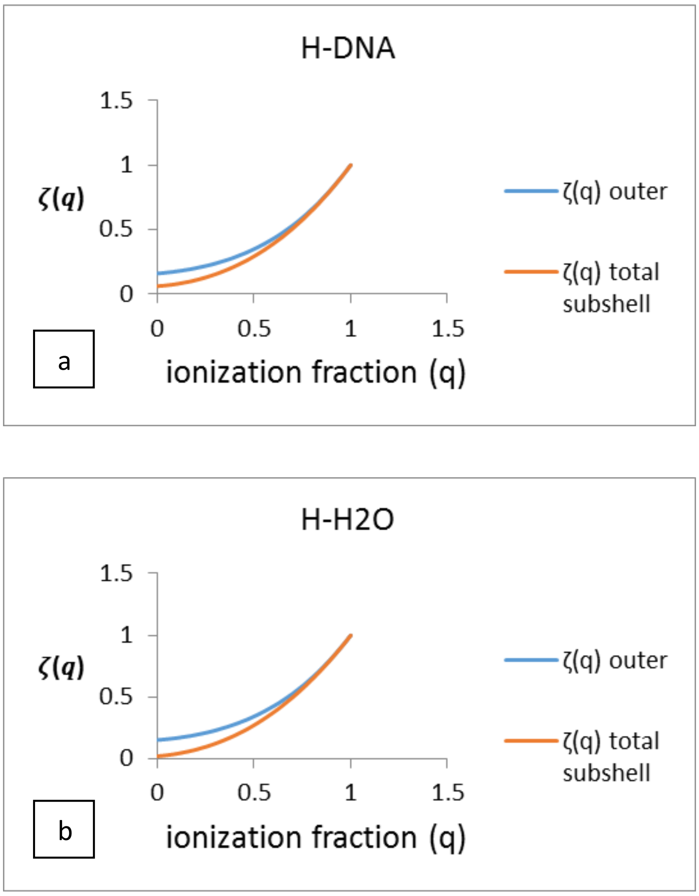
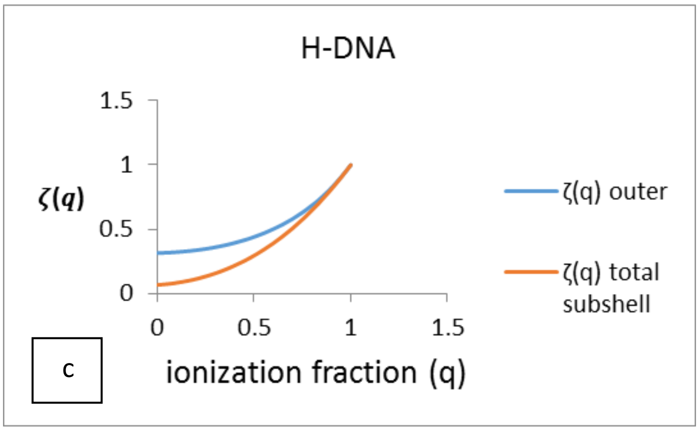


Fig. 1$\zeta(q)$ for proton in outer shell and total subshell of (a) DNA and (b) liquid water with ionization fraction (q)at incident energy $(T = 0.05\ \mathrm{MeV/u})$.



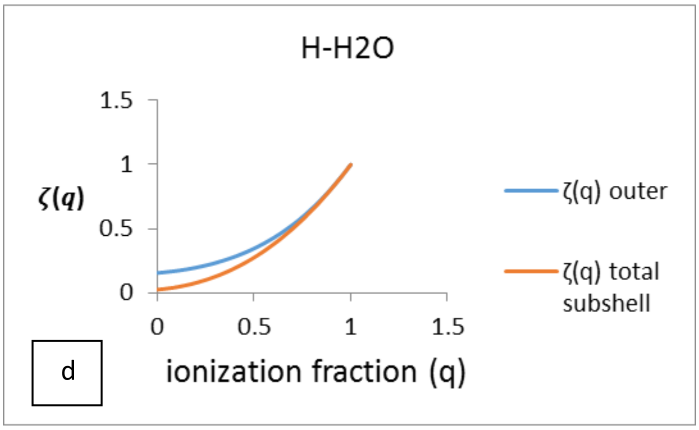


Fig. 2ζ(q) for proton in outer shell and total subshell of (c) DNA and (d) liquid water with ionization fraction (q)at incident energy $(\mathrm{T} = 0.25\ \mathrm{MeV/u})$.

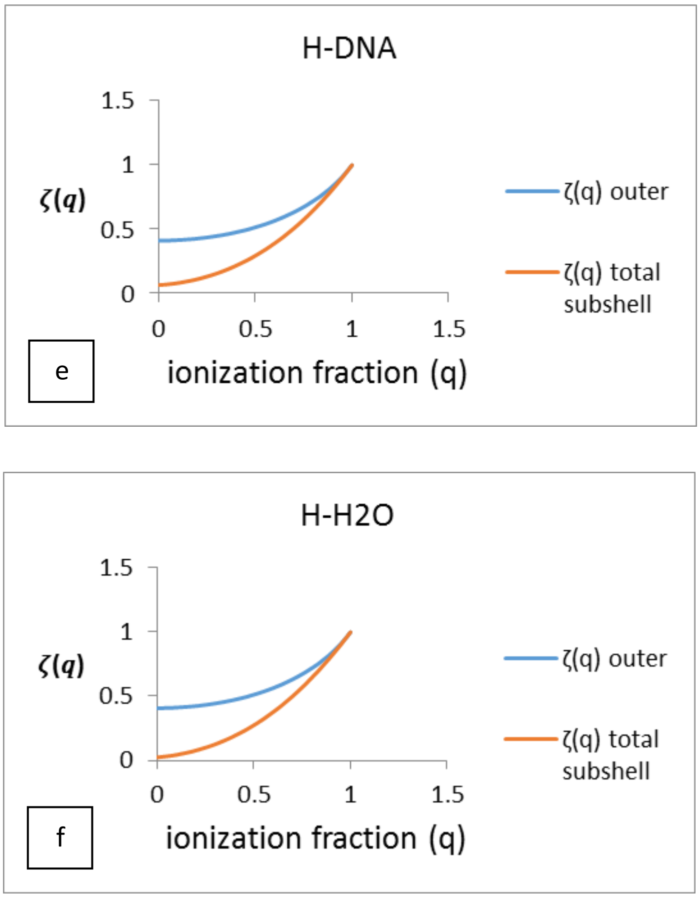
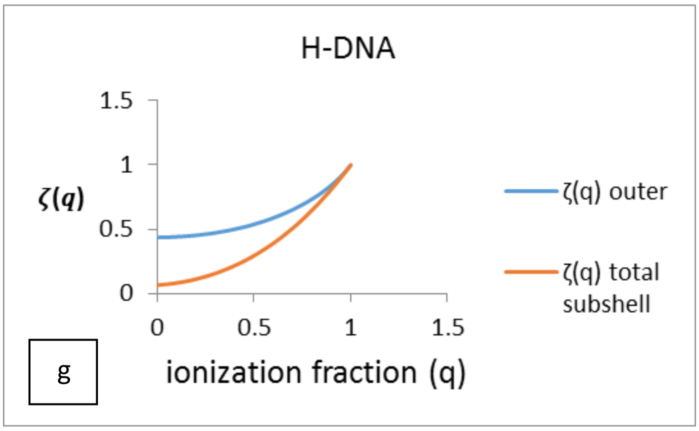


Fig. 3$\zeta(q)$ for proton in outer shell and total subshell of (e) DNA and (f) liquid water with ionization fraction (q)at incident energy $(T = 1\ \mathrm{MeV/u})$.



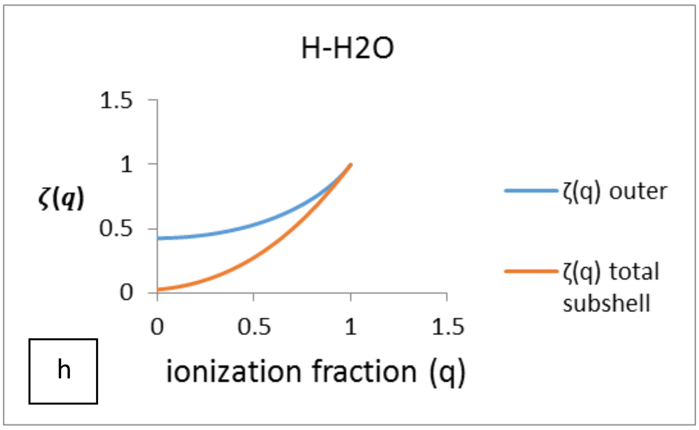
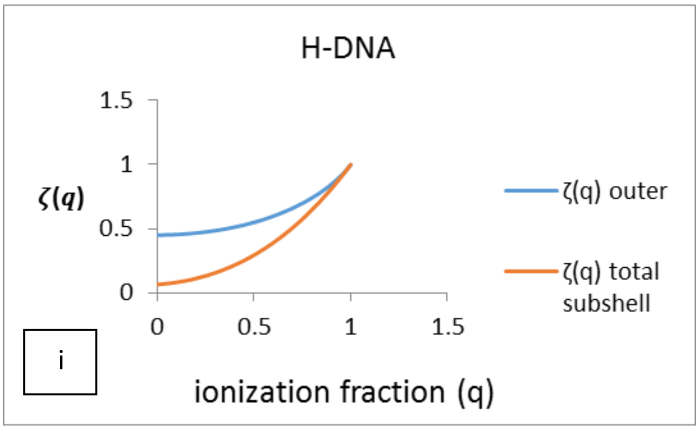


Fig. 4ζ(q) for proton in outer shell and total subshell of (g) DNA and (h) liquid water with ionization fraction (q)at incident energy $(\mathrm{T}=2\ \mathrm{MeV/u})$.



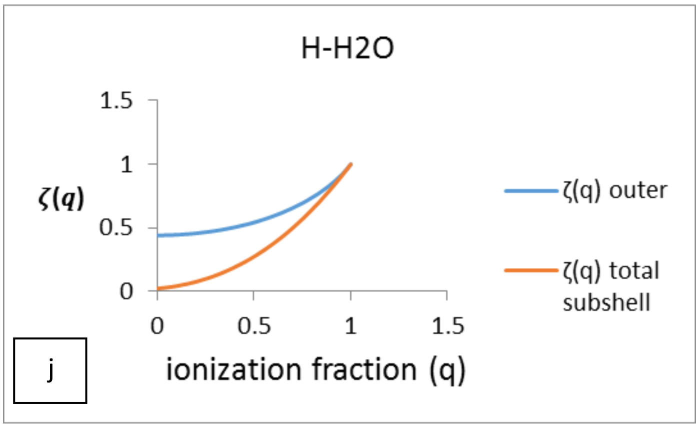


Fig. 5ζ(q) for proton in outer shell and total subshell of (i) DNA and (j) liquid water with ionization fraction (q)at incident energy (T = 2.5 MeV/u).