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# Convolution Approximation Method (CAM) for Energy Loss of Cluster Ions

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**الخلاصة**

ان فقدان الطاقة لجزيئة عنقودية كدالة لمعامل التصادم اقل معرفة نسبة الى فقدان الطاقة الذرية, كما ان تأثير معامل التجاور المتكون بالتداخل الذاتى مابين شضايا العنقود يلعب دورا رئيسيا فى حساب قدرة الايقاف الالكترونية للعنقود. فى هذا العمل استخدام عنقود الهايدروجين الثنائى فى هدف الهيدروجين باستخدام ثلاثة انواع من الجهود وهى كولوم و بور وزيتا-الاحادية وبعدة اتجهات. تم الحصول على توافق جيد مابين تقريب الالتفافية لجزيئة الاضطراب ( ) والتصادمات القريبة والقطبية عندما يكون معامل التصادم أقل أو يساوي أثنان .

**Abstract**

Electronic energy loss of molecular cluster as a function of impact parameters is less understood than atomic energy loss. Vicinage effect due to mutual interference between cluster fragments play a key role in the determination of the cluster electronic energy loss. In present work we used Hydrogen di-cluster ions in Hydrogen using three kinds of potentials, Coulomb, Bohr and single-zeta potentials at different orientations. Good agreement between molecular perturbation convolution approximation (MPCA), dipole and close collisions at impact parameter $p \leq 2$.

**1. Introduction**

Energy loss and channeling phenomena of molecular and cluster ions are not so well understood as the corresponding phenomena for mono-atomic ions. Important cluster beam applications can be found in the enhanced sputtering process [1-4], in secondary-electron emission enhancement [5], in plasma physics [6], and in inertial nuclear fusion [7] due to the vastly enhanced cluster energy deposition. The effects of a cluster clearly deviate from the sum of individual effects of each cluster component. In other words there is interference among the transitions induced by the different cluster components. This interference was shown for the ion energy loss [8]. The energy loss effects were extensively studied in a review paper [9] which describes the so-called vicinage effect, the non-additivety of the cluster component energy losses. While penetrating the target, a swift cluster ion loses a large fraction of its electrons and, then, undergoes a break process due to quasi-Coulomb forces among its components. If the clusters enter along a principal crystal axis, their motion will be guided due to the correlated collisions with the target atoms and, the motion of the molecule or its fragments will additionally depend on the Coulomb explosion.

A theoretical investigation of the cluster stopping power under channeling conditions requires the use of impact-parameter method [8]. The impact-parameter method describes the energy loss $\Delta E(p)$ between the projectile and the target as a function of the impact parameter $p$, namely $\Delta E(p)$, for a classical projectile trajectory.

This work describes an extension of the perturbative convolution approximation (PCA) model [5,10], based on the impact-parameter method, for molecules and clusters, namely MPCA. MPCA gives the energy loss as a function of impact-parameter without time consuming first-order calculations using a set of thousands of final states for both distant- and close collisions. The starting point of the model is the diatomic molecule. The physical inputs of the model are the target oscillator strengths, the target electronic density, the projectile screening function and the molecular alignment angles [11].

## 2. Theory

### 2.1 Molecular perturbation convolution approximation (MPCA)

The MPCA model is an extension of PCA model [5,10] made for cluster projectiles, and according to the outline of PCA given [12], a special attention must be pay to the interference terms that arise from the sum of all ionic potential. In order to calculate the energy loss due to target ionization and excitation we have to consider the amplitude for each electronic transition from the ground-state $|0\rangle$ with energy $\varepsilon_0$ to a final state $|f\rangle$ with energy $\varepsilon_f$ [12, 13]. Thus Eq. (1) in [12] becomes,

$$a_f = -i\int_{-\infty}^{\infty} dt\, e^{i(\varepsilon_f-\varepsilon_0)t}\,\langle f|\sum_i^N V_i\left(\vec{r}-\vec{R}_i(t)\right)|0\rangle, \qquad 1$$

Where $V_i$ is the interacting potential between the *ith.* Ion (whose charge is $Z_i$) in the cluster and the target electron. The *ith.* ion position in space is $\vec{R}_i(t)$ and $\vec{r}$ is the target electron coordinate, both relative to the target nucleus.

The time of interaction between the cluster and the target is much smaller than the characteristic times of vibrational and rotational cluster transitions. Therefore, the corresponding degree of freedom can be neglected. The time dependent position of the *ith.* projectile nucleus is given by $\vec{R}_i(t)=\vec{p}_i+vt+d_{iz}$, where $\vec{d}_i$ is the distance between the molecule center and the *ith* ion, $\vec{d}_{iz}$ is the z-component of $\vec{d}_i$, $\vec{d}_{i\rho}$ is the transversal component of $d_i$ and $\vec{p}_i=\vec{p}+\vec{d}_{i\rho}$ which is the *ith* ion impact parameter as shown in Fig. (1). The angle $\vartheta$ in Fig.(1) refers to the angle between the

diatomic molecule axis and the z-axis, and the angle $\phi$ refers to the angle between $\vec{d}_{i\rho}$ and the x-axis [11,14].

At large impact parameters the dipole approximation for $V_i\left(\vec{r}-\vec{R}(t)\right)$ can be used, where [15],

$$V\left(\vec{r}-\vec{R}(t)\right)\approx V\left(\vec{r}-\vec{R}(t)\right)_{r=0}+\vec{r}.\vec{\nabla}_r V\left(\vec{r}-\vec{R}(t)\right)_{r=0} \qquad (2)$$

And the expression of energy loss [13],

$$\Delta E^{dipol}(p)=\sum_{i=1}^{N}\Delta E^{dipol}_{atomic}(\vec{p}_i)+\sum_{i=1}^{N}\sum_{j>1}^{N}\Delta E^{dipol}_{\text{int}}(\vec{p}_i,\vec{p}_j), \qquad (3)$$

Where

$$\Delta E_{\text{int}}^{dipol}\left(\vec{p}_i,\vec{p}_j\right)=\sum_{\beta} f_\beta \frac{2Z_iZ_j}{\upsilon^2}\cos\left(\frac{\omega_{\beta 0}d_{ijz}}{\upsilon}\right)$$

$$X \quad \left[\frac{2\vec{p}_i\cdot\vec{p}_j}{\left(p_ip_j\right)^2}g_\perp(p_i)g_\perp\left(p_j\right)+\frac{2g_{11}(p_i)g_{11}\left(p_j\right)}{p_ip_j}\right] \tag{4}$$

Where, for the Coulomb potential, the functions $g_{11}(p_i)$ and $g_\perp(p_i)$ read [5,16]

$$g_{11}(p_i)=\left(\frac{\omega_{\beta 0}p_i}{\upsilon}\right)K_0\left(\frac{\omega_{\beta 0}p_i}{\upsilon}\right) \tag{5}$$

And

$$g_\perp(p_i)=\left(\frac{\omega_{\beta 0}p_i}{\upsilon}\right)K_1\left(\frac{\omega_{\beta 0}p_i}{\upsilon}\right), \tag{6}$$

Where $K_0(x)$ and $K_1(x)$ are second kind Bessel functions, $d_{ijz}=d_i\cos\vartheta_i-d_j\cos\vartheta_j$ and $\vartheta_i$ is the angle between the z-axis and $\vec{d}_i$. The

first term in Eq. (3) corresponding to the individual $\Delta E_{atomic}^{dipol}(p)$ associated to each ion and the second term is associated to interference effects (vicinage).

$$p_i=p_j+d_i\sin\vartheta_i+d_j\sin\vartheta_j,$$
$$p_j=p_i-d_i\sin\vartheta_i-d_j\sin\vartheta_j,$$

Thus,

$$\frac{2(p_i, p_j)}{(p_i p_j)^2} = \frac{2}{p_j^2} - \frac{2d_{i\rho}\cos\phi}{p_i p_j^2} - \frac{2d_{j\rho}\cos\phi}{p_i p_j^2}\ , \qquad (7)$$

Where, $d_{i\rho} = d_i \sin\vartheta_i$ ; $d_{j\rho} = d_j \sin\vartheta_j$

For $d_i = d_j = d$ and $\vartheta_i = \vartheta_j = \vartheta$,

Then,

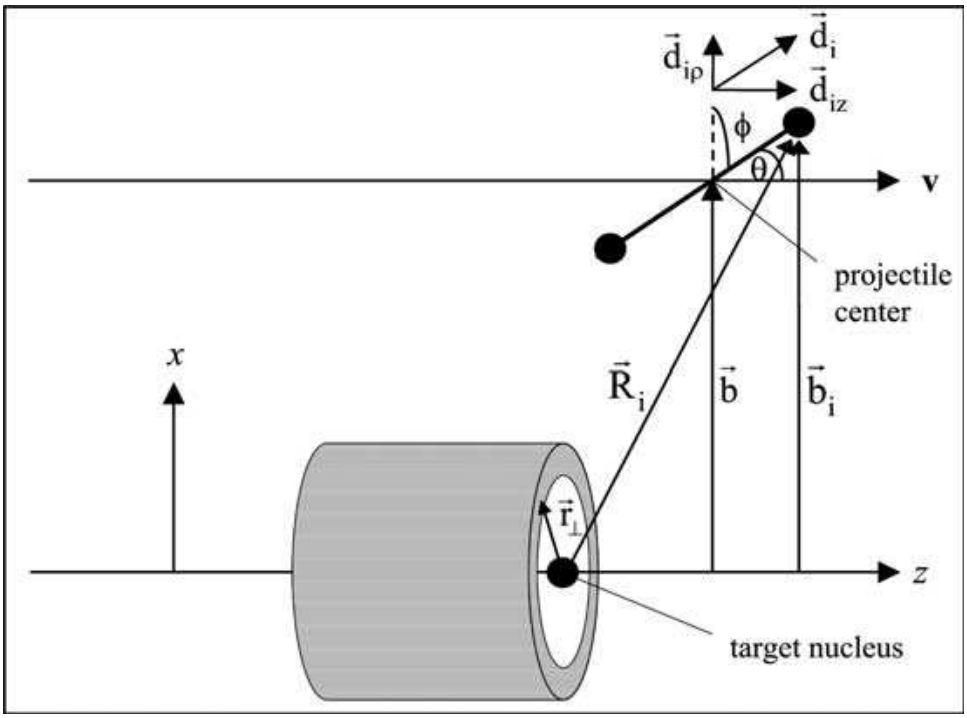



Fig.(1) Schematic plot of the collision geometry. Depicted are the structured projectile with its center, the target nucleus, the target-

electron density (integrated along z-axis), the relevant impact parameters, the projectile vectors $\vec{d}$ and for a diatomic projectile, the characteristic orientation angles $\vartheta$ and $\phi$. The inset shows a front view of the molecule, in order to clarify the meaning of the angle $\phi$ [14].

$$\frac{2(p_i.p_j)}{(p_i p_j)^2}=\frac{2}{p_j^2}-\frac{4d_{i\rho}\cos\phi}{p_i p_j^2}=\frac{2}{p_j^2}\left[1-\frac{2d_{i\rho}\cos\phi}{p_i}\right] \tag{8}$$

For small impact parameters, the influence of the target potential can be neglected at high projectile energies allowing for an analytical expression for $\Delta E^{close}(p)$ by replacing the final target continuum states by plane waves (see chapter (3) [13]). Thus, the energy transfer reads

$$\Delta E^{close}(p)=\sum_{i=1}^{N}\Delta E_{atomic}^{close}(\vec{p}_i)+\int d^2 r_\perp T_{\text{int}}^{close}(\vec{r}_\perp-\vec{p})\int_{-\infty}^{\infty} dz\rho(\vec{r}_\perp,z), \tag{9}$$

Where $\rho$ is the electronic target density.

The first term corresponds to a incoherent sum of energy losses due to each ion from the cluster and,

$$T_{\text{int}}^{close}(\vec{p})=\frac{2}{\upsilon^2}\sum_{i=1}^{N}\sum_{j>1}^{N} Z_i Z_j h_{\text{int}}(\vec{p}_i,\vec{p}_j) \tag{9}$$

Is the interference term [11],

$$h_{\text{int}}(\vec{p}_i,\vec{p}_j)=4\upsilon^2\int_0^1 dqq^2\cos(\beta d_{ijz})\Big\{q\Big[j_0\left(\alpha p_i\sqrt{1-q^2}\right)K_0(\beta p_j)+j_0\left(\alpha p_j\sqrt{1-q^2}\right)K_0(\beta p_i)\Big]$$
$$+\sqrt{1-q^2}\frac{\vec{p}_i}{p_i}\frac{\vec{p}_j}{p_j}\Big[K_1(\beta p_j)j_1\left(\alpha p_i\sqrt{1-q^2}\right)+K_1(\beta p_i)j_1\left(\alpha p_j\sqrt{1-q^2}\right)\Big]\Big\} \tag{11}$$

Where $\alpha = 2\upsilon q$, $\beta = 2\upsilon q^2 = \alpha q$, $j_0$ and $j_1$ are zero and first order of first kind Bessel functions.

According to the discussion of the function $h(x)$ given in [12], the function $h_{\text{int}}(\vec{p}_i, \vec{p}_j)$ approaches to zero for $p_i << 1/\upsilon$ or $p_j << 1/\upsilon$ and, for large values of $p$ (i.e large values for both $p_i$ and $p_j$), it reaches

$$h_{\text{int}}(\vec{p}_i, \vec{p}_j) \approx 2\frac{\vec{p}_i \cdot \vec{p}_j}{(p_i p_j)^2}, \tag{12}$$

Recognized as the interference part of the classical sudden approximation result [4] for a diatomic molecule.

Now, to propose a general formula apply for all impact parameters ,

$$\Delta E(p) = \int d^2 r_\perp T_{MPCA}(\vec{r}_\perp - \vec{p}) \int_{-\infty}^{\infty} dz\, \rho(\vec{r}_\perp, z) \tag{13}$$

Where the function $T(\vec{p})$ for the cluster can be written as a sum of the energy losses due to each individual ion from the cluster as presented in chapter three for a single ion projectile $T_{atomic}^{PMCA}$ and the interference part which is the correlated part between two ions $T_{\text{int}}^{PMCA}(\vec{p})$, thus:

$$T_{PMCA}(\vec{p}) = T_{atomic}^{PMCA}(\vec{p}) + T_{\text{int}}^{PMCA}(\vec{p}), \tag{14}$$

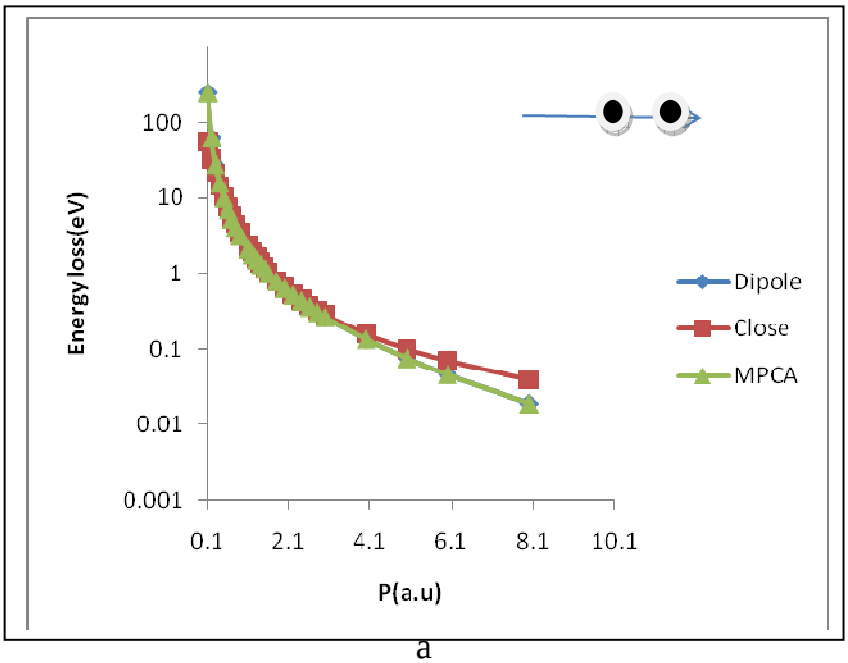
$$T_{\text{int}}^{MPCA}(\vec{p}) = \sum_{\beta} f_\beta \sum_{i=1}^{N} \sum_{j>1}^{N} \frac{2Z_i Z_j}{\upsilon^2} \cos\left(\frac{\omega_{\beta 0} d_{ijz}}{\upsilon}\right)$$
$$X \quad \left[ h_{\text{int}}(2\upsilon\vec{p}_i, 2\upsilon\vec{p}_j) g_\perp(p_i) g_\perp(p_j) + \frac{2 g_{11}(p_i) g_{11}(p_j)}{\sqrt{p_i^2 + p_{\min}^2}\sqrt{p_j^2 + p_{\min}^2}} \right] \tag{15}$$

Where $p_{\min} = 1/v^2$ is defined in [15]. This is the molecular perturbative convolution approximation (PMCA).

3. Results and discussion

The cluster under consideration will be the diatomic hydrogen molecule and the angles $\vartheta$ and $\phi$ are shown in Fig.(1). Figs.(2-10) show the comparison between dipole and close collision interference terms with the corresponding MPCA for di-cluster atomic hydrogen ions in hydrogen target at different orientation. The numerical calculations has been done using a program $ghscren1s.f90$ which has been written in FORTRAN-90 using the software Compaq visual Fortran (CVF) for compiling, linking and executing the program. For both orientations, the MPCA and close-collision interference terms agree with each other for small impact parameters and the same is observed between MPCA and dipole-approximations for large impact parameters, thus reinforcing the validity of general formula Eq.(3.12) [13]. It should be stressed that sudden approximation, which is link close- and distant collisions for atomic projectiles, in fact does not link the interference term for close and distant collisions properly. This comes from the fact that classical sudden approximation does not contain the interference term due to the phase difference along the z-direction (e.g. the cosine term in Eqs. (4-6).

In Figs. (2-10) the MPCA agree with close and distant collisions at impact parameter $p \le 2$ for Coulomb, Bohr and single-zeta potentials. There are two cases: (i) molecule has no bound electrons (two protons traveling together, interacting with Coulomb forces) and (ii) one of the proton has captured one electron from medium ( $H^+$ and $H^0$ traveling together) [11]. The two ions will have a head-on-collision with target at $\vartheta = 0$ and $\phi = 0$, where the molecules axis perpendicular to the impact parameter and parallel to its motion. For $\vartheta = 90$ and $\phi = 0$ the molecule has its axis orthogonal to its motion and parallel to the impact parameter direction, the increase of energy loss up to impact-parameter about 1 a.u. is due the choice of the coordinated system. In that orientation and for $p = 1 a.u$, one of the ions (namely the second) will have a head-on-collision with the target. For $\vartheta = 90$ and $\phi = 90$ the molecule has its axis orthogonal to its motion and impact-parameter direction, the increase of energy loss up to impact-parameter approach to zero. In all orientation, the effect of interference terms leads at an increase in energy loss of about 50% for distant-collisions and less than 10% for close-collisions. That results agrees with the united-atom model for the distant-collisions, where the energy loss is proportional to $(Z_1 + Z_2)^2$ (4, for $H_2^+$) and independent atom model for close-collisions, where $S_c$ is proportional to $\left(Z_1^2 + Z_1^2\right)$ (2, for $H_2^+$).

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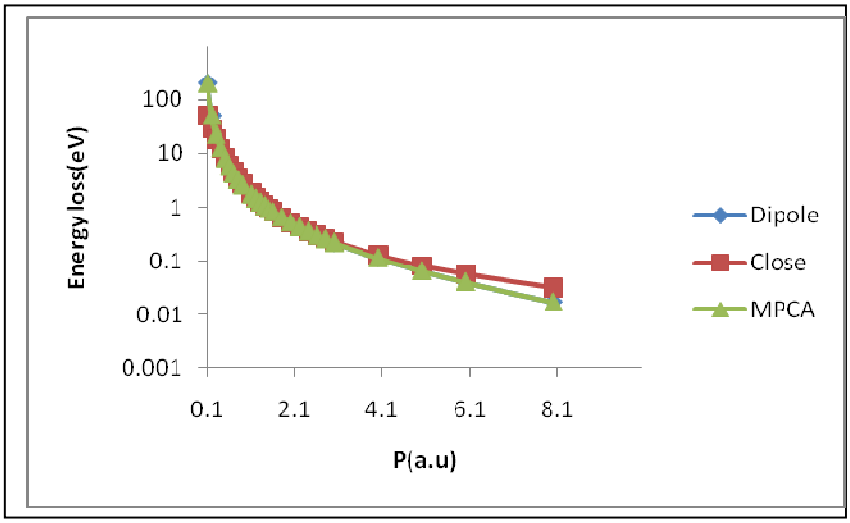


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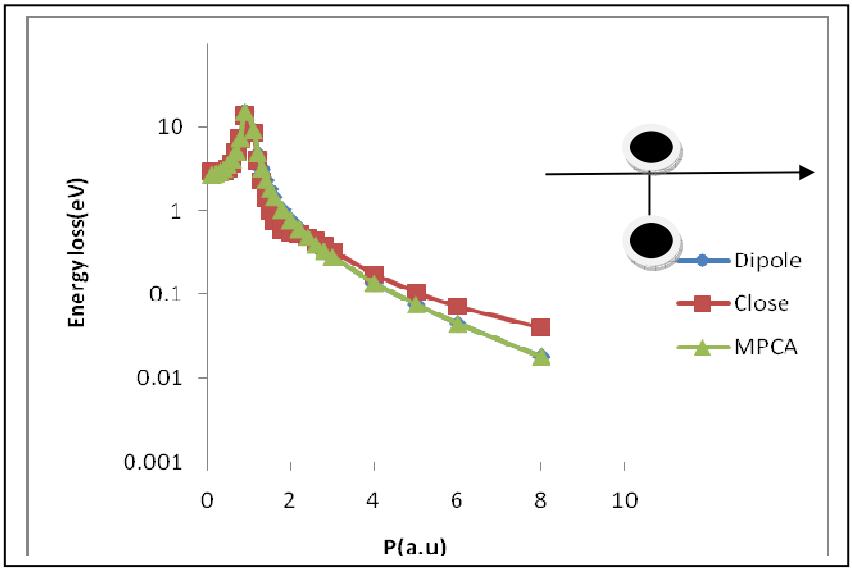
Fig.(2 ) Comparison between dipole, close collisions and MPCA model of Coulomb potential for energy loss (eV) of di-cluster hydrogen ions at angles $\vartheta = 0$ and $\phi = 0$ in hydrogen at (a) 400keV (b) 500keV.

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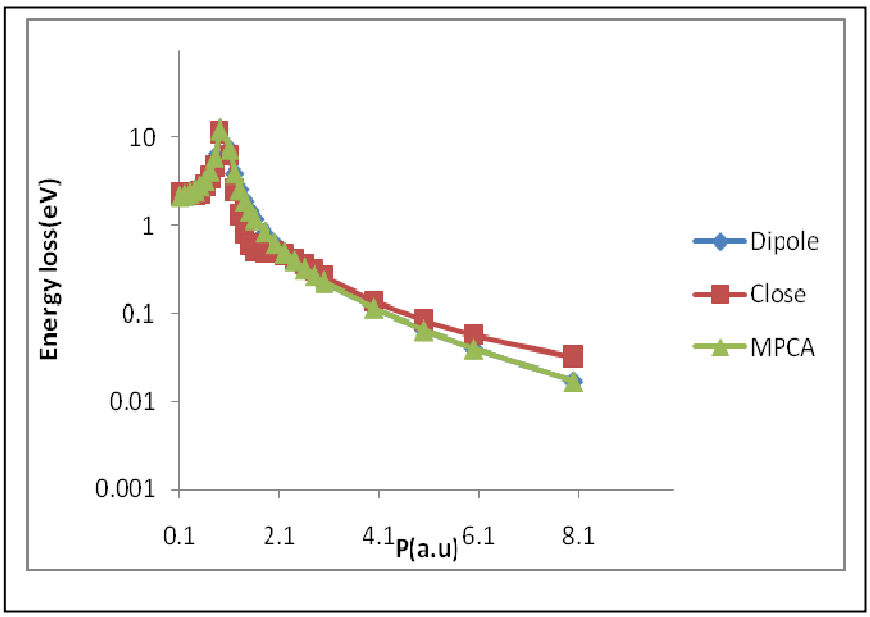


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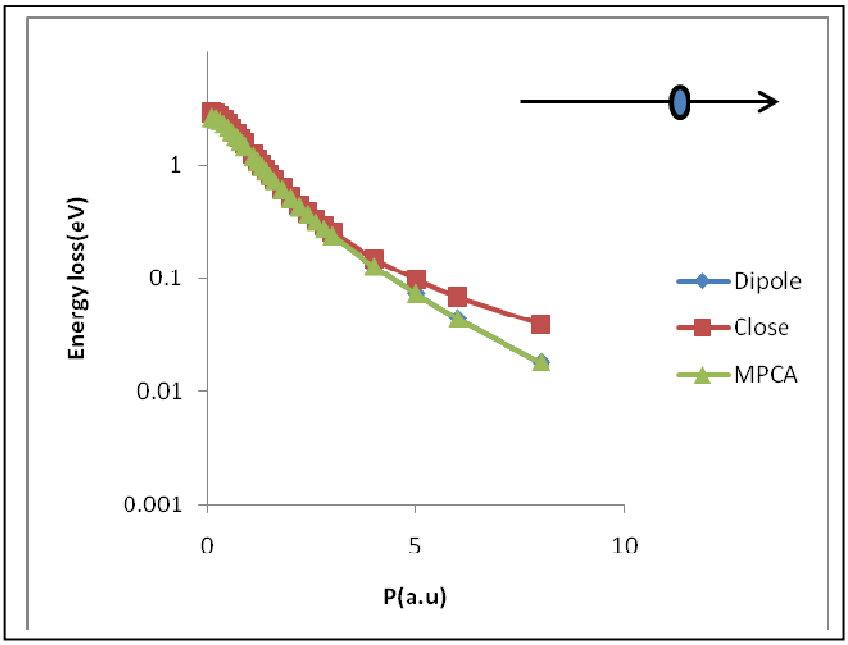
Fig.(3 ) Comparison between dipole, close collisions and MPCA model of Coulomb potential for energy loss (eV) of di-cluster hydrogen ions at angles $\vartheta = 90$ and $\phi = 0$ in hydrogen at (a) 400keV (b) 500keV.

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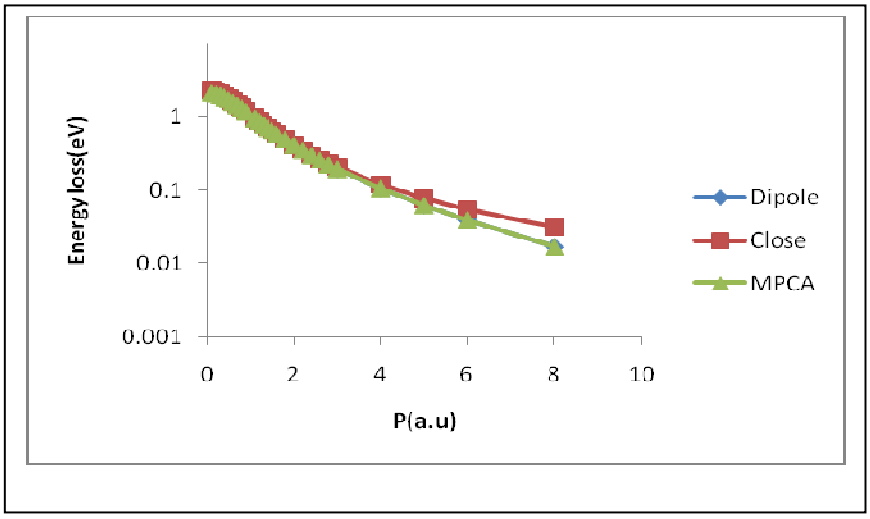


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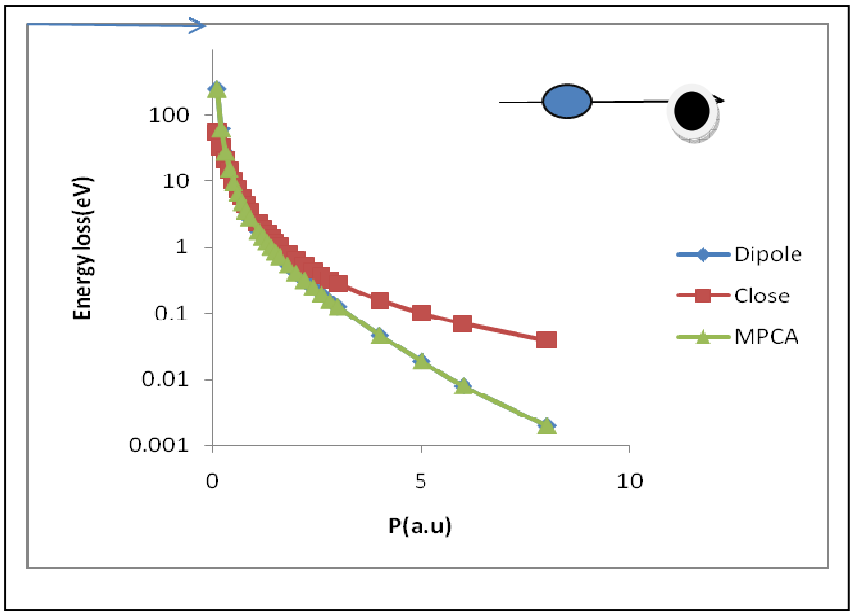
Fig.(4 ) Comparison between dipole, close collisions and MPCA model of Coulomb potential for energy loss (eV) of di-cluster hydrogen ions at angles $\vartheta = 90$ and $\phi = 90$ in hydrogen at (a) 400keV (b) 500keV.

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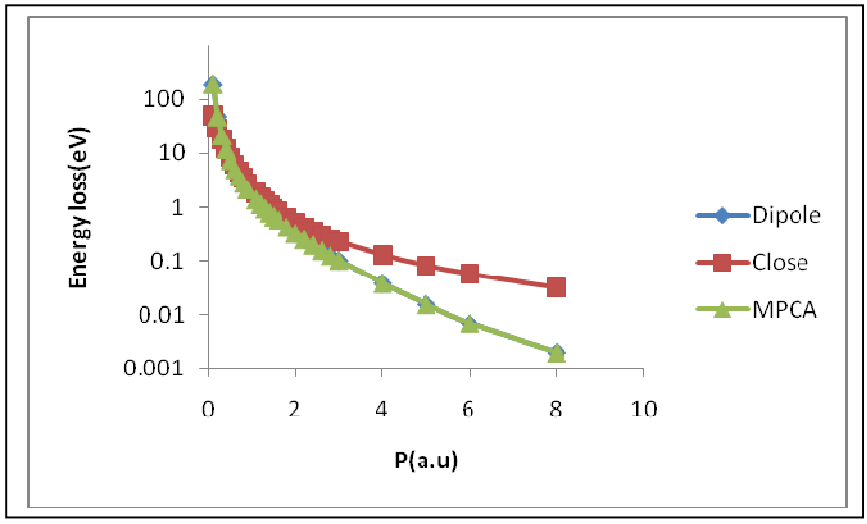


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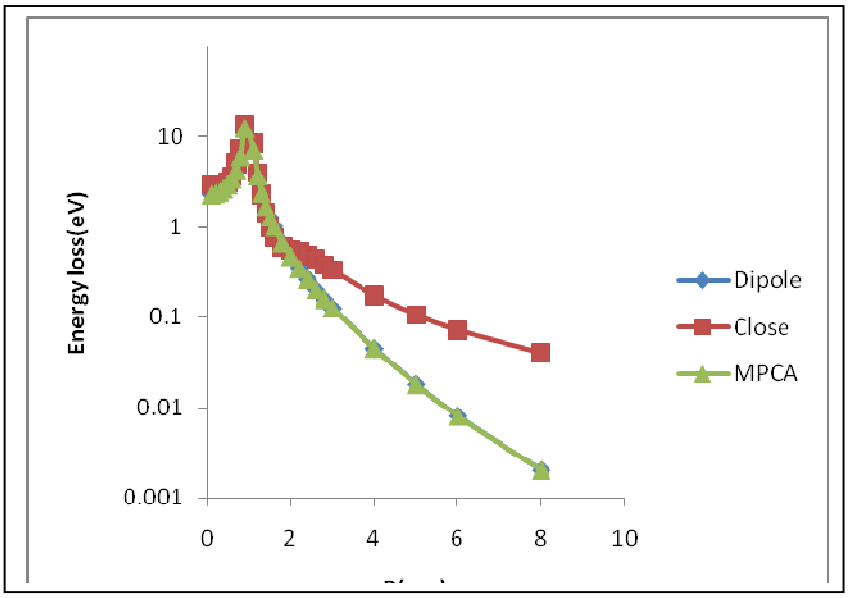
Fig.(5 ) Comparison between dipole, close collisions and MPCA model of Bohr potential for energy loss (eV) of di-cluster hydrogen ions at angles $\vartheta = 0$ and $\phi = 0$ in hydrogen at (a)400keV (b)500keV.

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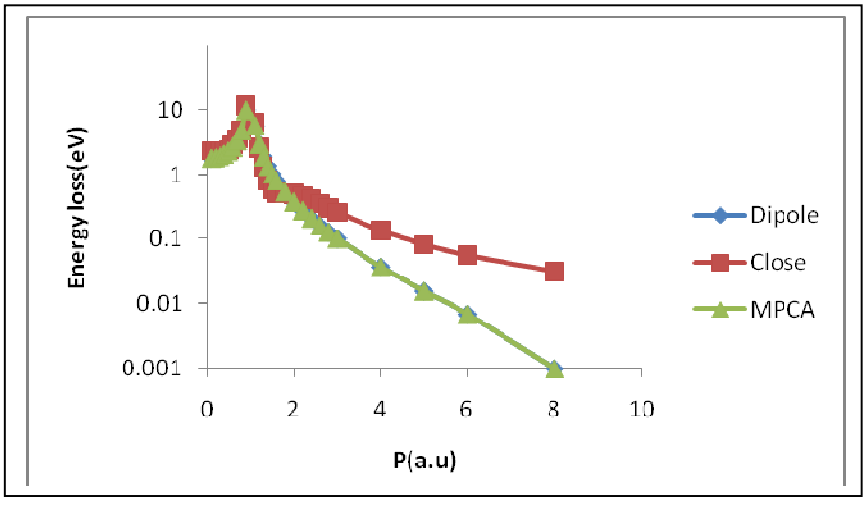


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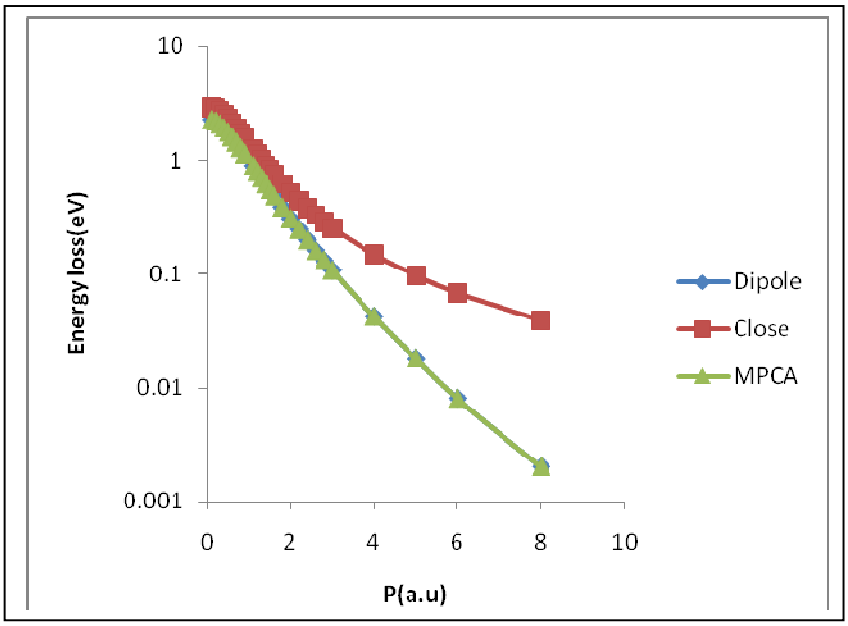
Fig.(6 ) Comparison between dipole, close collisions and MPCA model of Bohr potential for energy loss (eV) of di-cluster hydrogen ions at angles $\vartheta = 90$ and $\phi = 0$ in hydrogen at (a)400keV (b)500keV.

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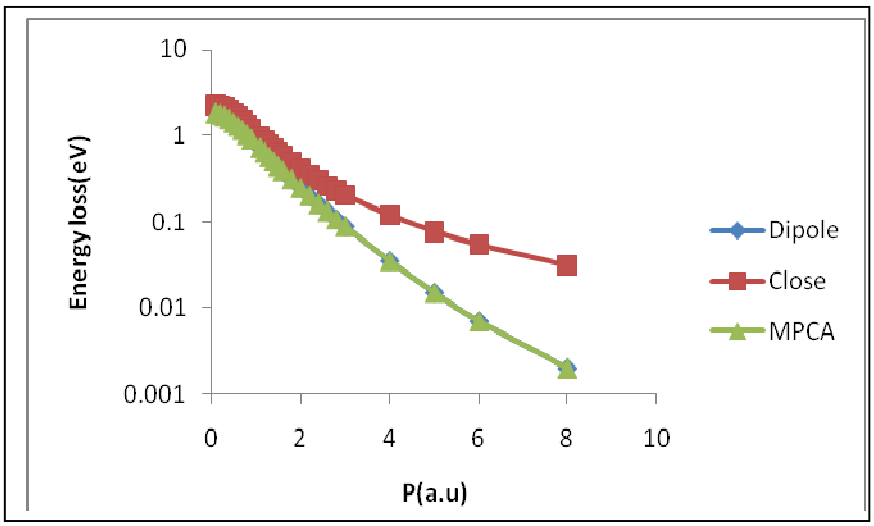


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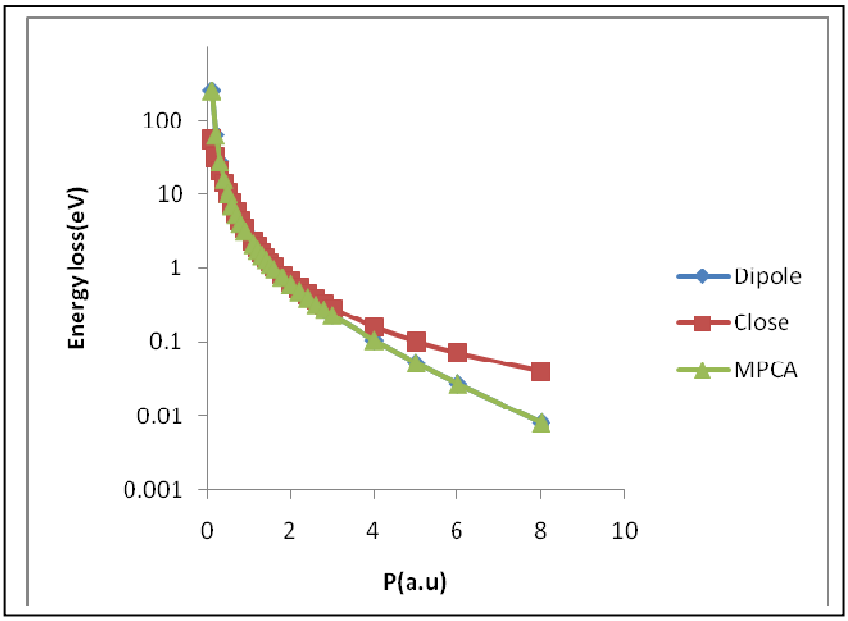
Fig.(7 ) Comparison between dipole, close collisions and MPCA model of Bohr potential for energy loss (eV) of di-cluster hydrogen ions at angles $\vartheta = 90$ and $\phi = 90$ in hydrogen at (a) 400keV (b) 500keV.

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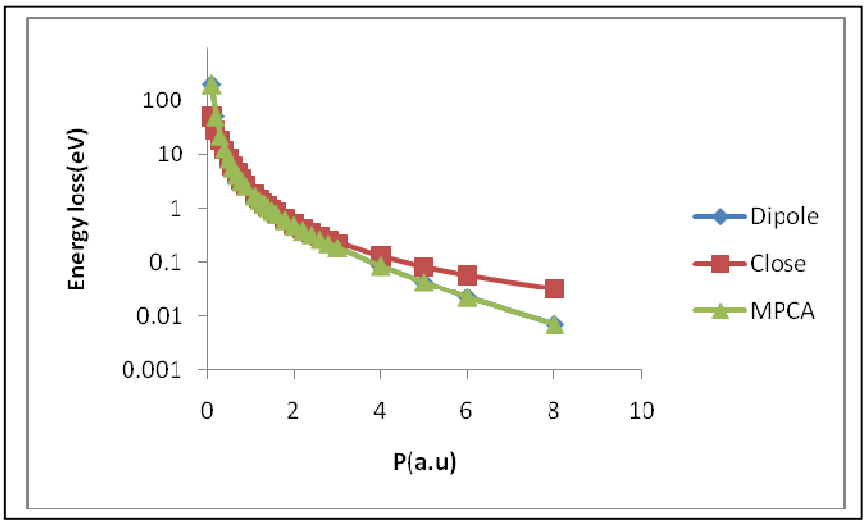


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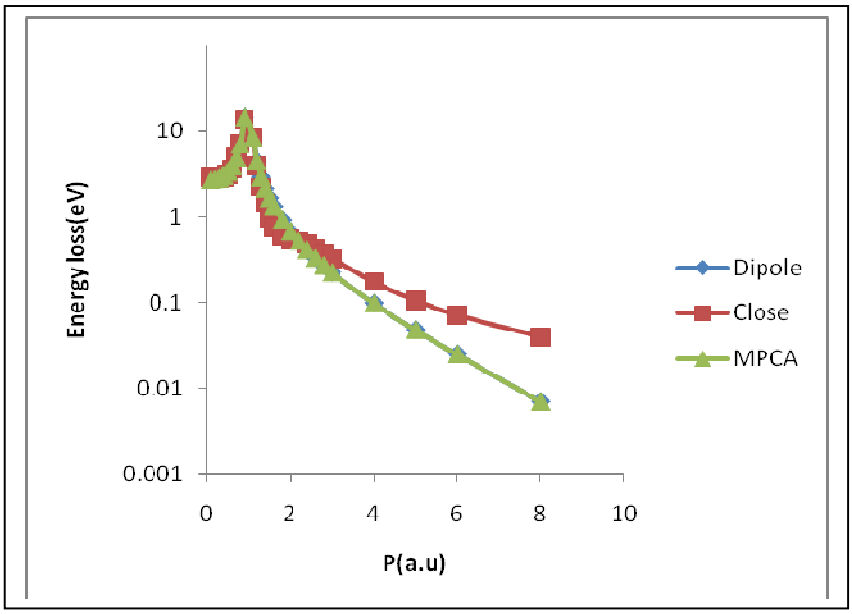
Fig.(8 ) Comparison between dipole, close collisions and MPCA model of single-zeta potential for energy loss (eV) of di-cluster hydrogen ions at angles $\vartheta = 0$ and $\phi = 0$ in hydrogen at (a) 400keV (b) 500keV.

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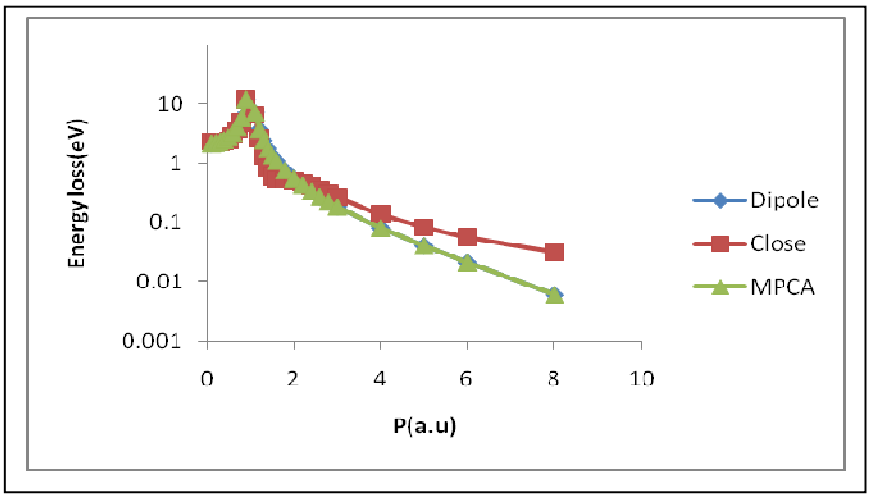


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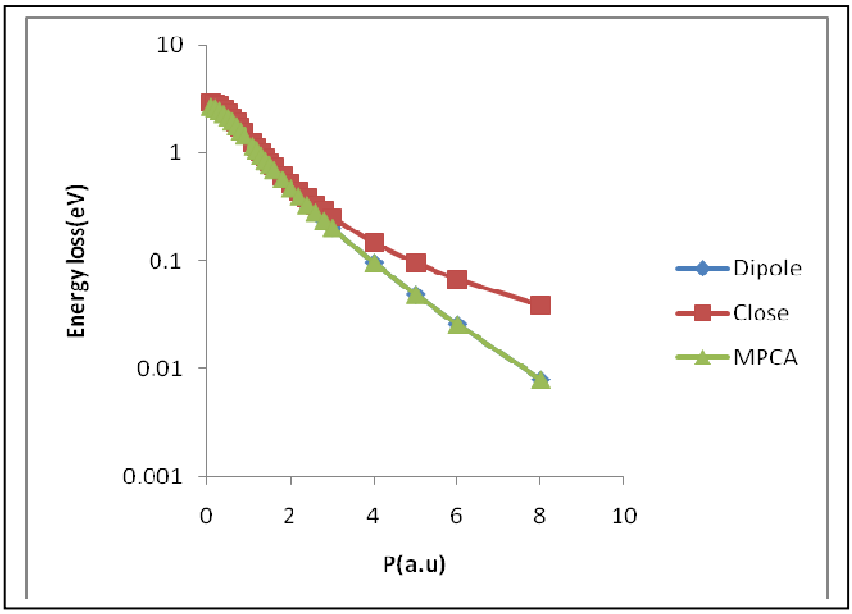
Fig.(9 ) Comparison between dipole, close collisions and MPCA model of single-zeta potential for energy loss (eV) of di-cluster hydrogen ions at angles $\vartheta = 90$ and $\phi = 0$ in hydrogen at (a) 400keV (b) 500keV.

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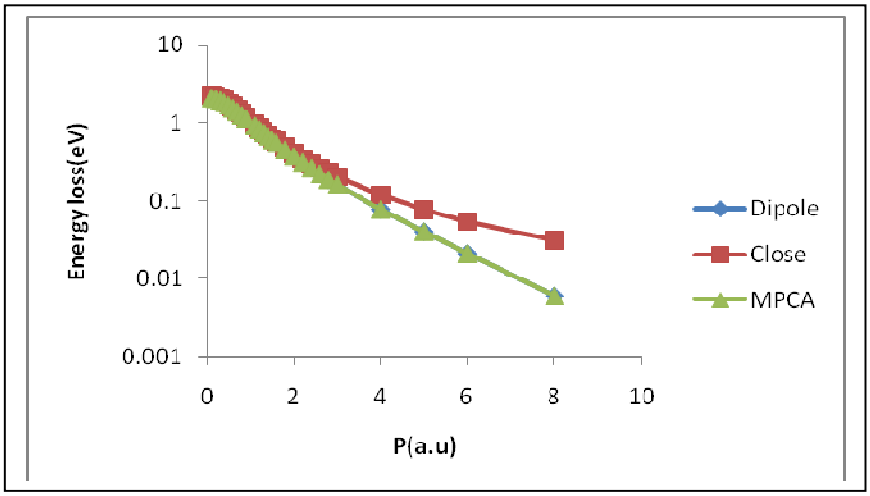


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Fig.(10 ) Comparison between dipole, close collisions and MPCA model of single-zeta potential for energy loss (eV) of di-cluster hydrogen ions at angles $\vartheta = 90$ and $\phi = 90$ in hydrogen at (a) 400keV (b) 500keV.

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