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Multiple Ionization of Atoms by Heavy Ions

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Independent Electron Model

Simple alternative approach, many electron system, based on LPA

Simple processes: ionization, stopping, straggling,...

Complex systems: molecules, solids, surfaces...

Complex problems: multiple ionization, antiscreening, induced potential

Talk 1- collision with surfaces

2- moments: Straggling, stopping & ionization X sect.

3- Multiple ionization of atoms

4- Advantages & disadvantages

Stopping (PRA 69, 062903 (2004), 73, 024901 (2006)).

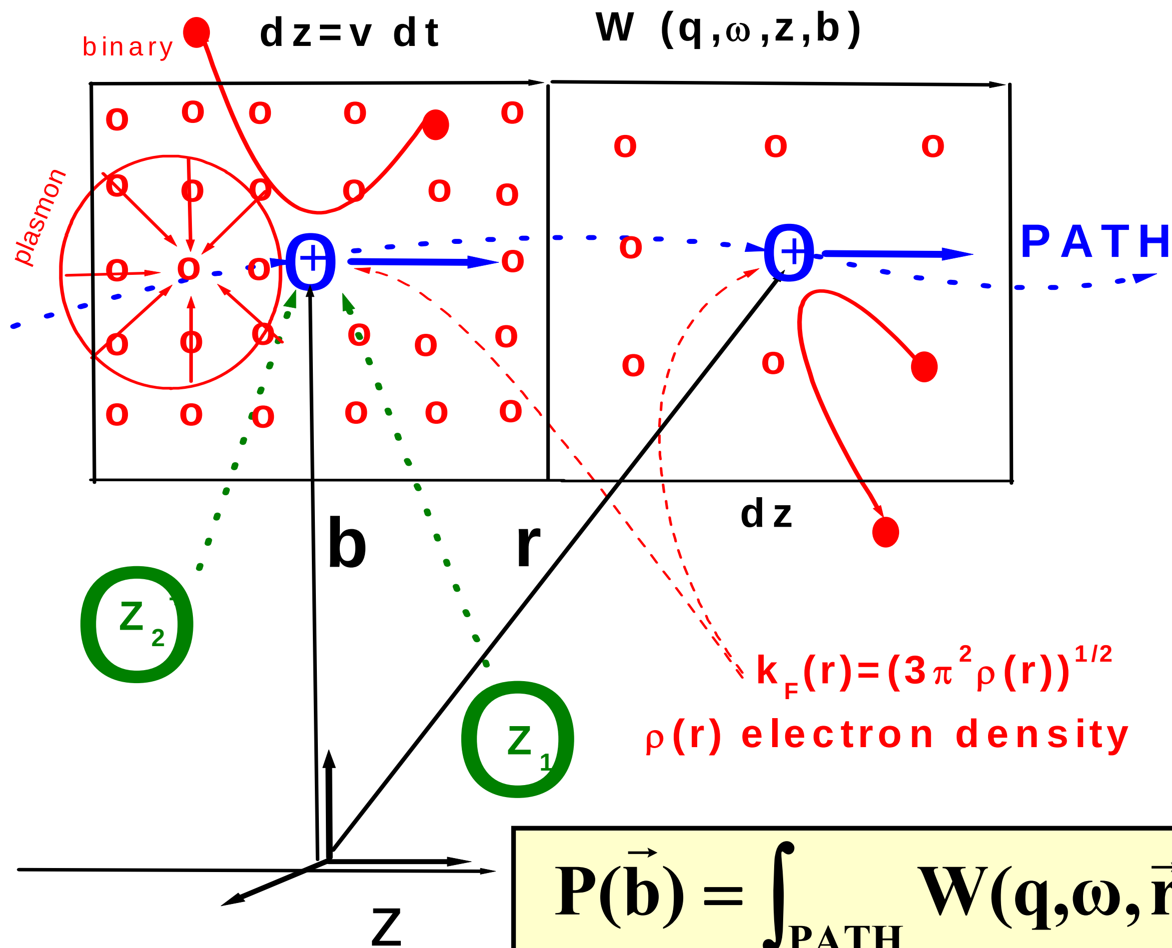
Straggling (PARA 75, 022903 (2007)).

Antiscreening (PRA 67, 062702 (2003)) .

Ionization (PRA 67, 032703 (2003), JPB 36 ,13043 (2003)).

On surfaces (PRA 74, 012902 (2006), 75, 042904 (2007)).

Local Plasma Approximation - LPA



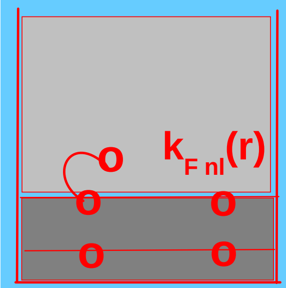
$$P(\vec{b}) = \int_{PATH} W(q,\omega,\vec{r})\, d\omega\, dq\, d\vec{z}$$

Lindhard *et al* (1953, 67), Brandt-Lundqvist (1966, 1967, 1970),

Bonderup (1967), Chu *et al* (1970, 1972)

DIELECTRIC RESPONSE FUNCTION

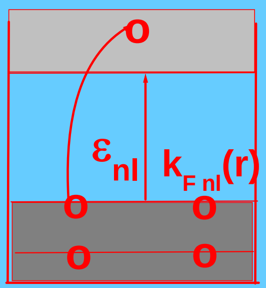
$$W(q,\omega,\vec{r}) = \frac{2Z_P^2}{\pi v^2}\frac{1}{q}\,\mathrm{Im}\left[\frac{1}{\varepsilon(q,\omega,k_F(\delta(\vec{r})))}\right]$$



$\varepsilon(q,\omega,k_F)$, $k_F = k_F(r)$, **Lindhard (1954),**

it accounts e - e correlation to all orders

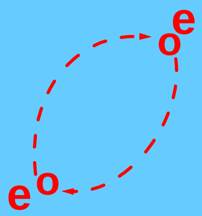
& Z_P to first order



$\varepsilon(q,\omega,k_F,\omega_{nl})$ **Levine & Louie (1982)**

$\uparrow$ **to account for the gap & f-sum rule**

shell-to-shell $\Rightarrow$ independent shell app.

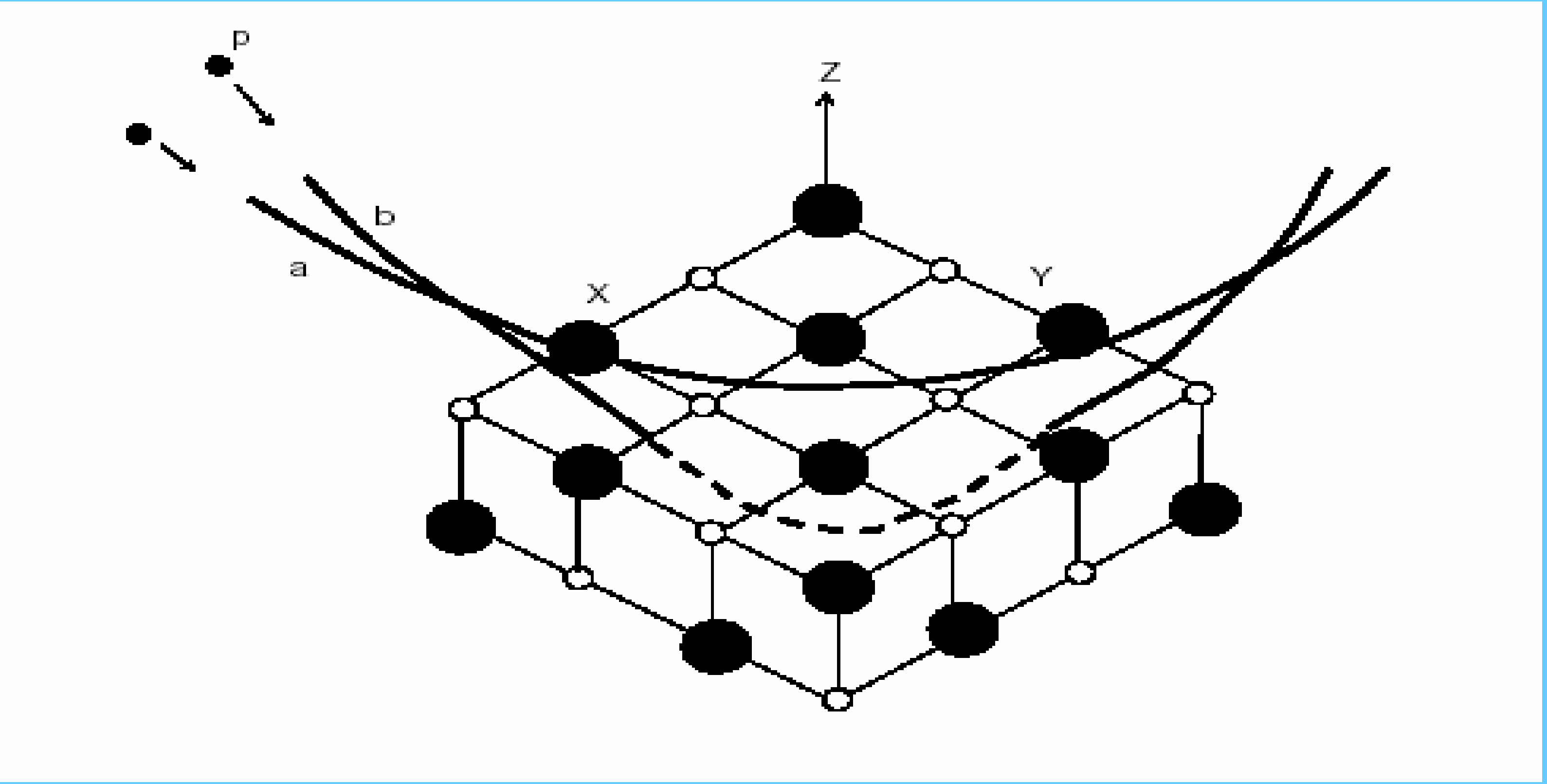


$\varepsilon(q,\omega,k_F,\omega_{nl},S(q))$ **Singwi (1968 – 1981)**

$\uparrow$ **to account for e - e exchange & pair**

2 – 3% no more

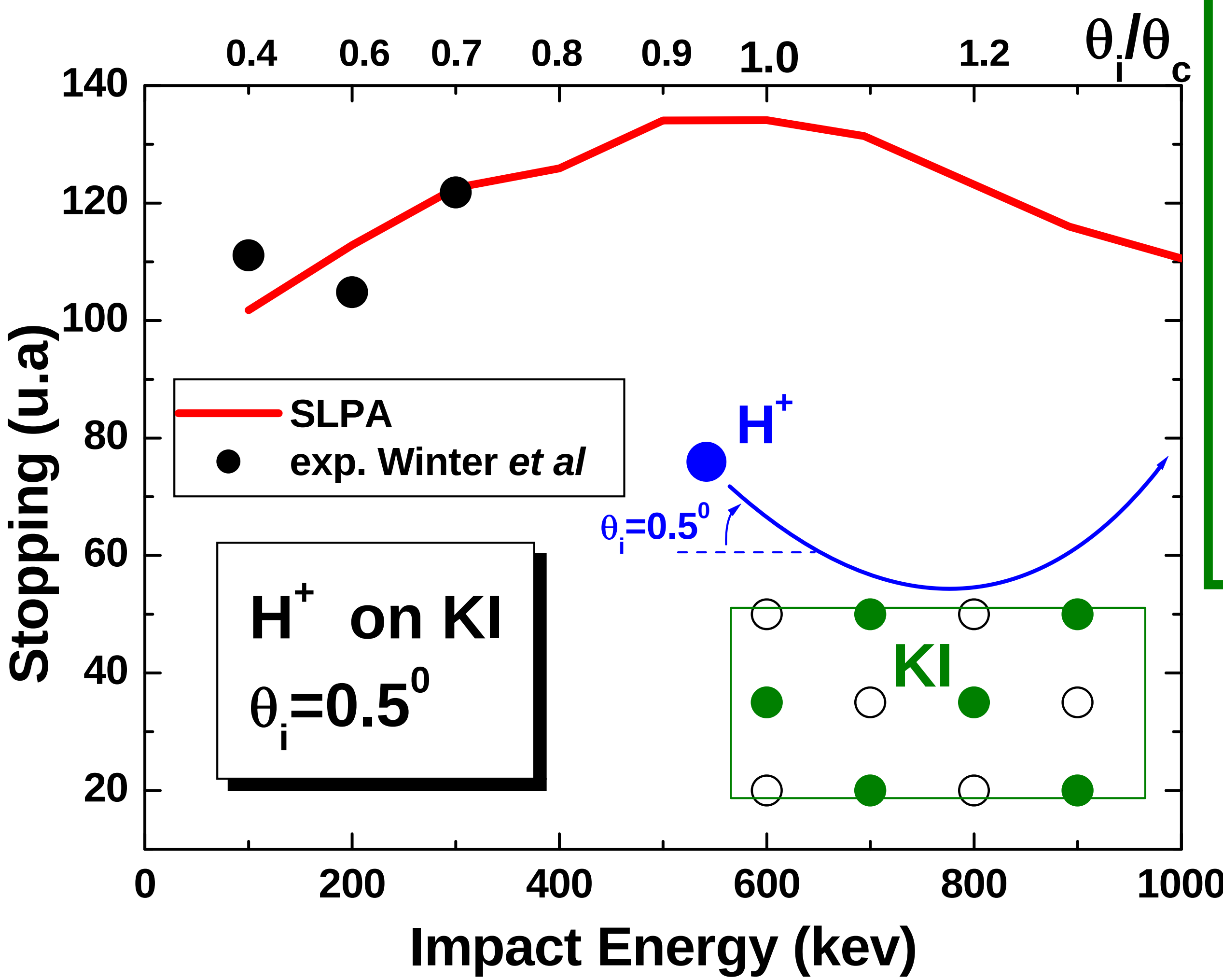
Collisions with insulator surfaces



16 insulators :

Li^+ , Na^+ , K^+ , Rb^+ with F^- , Cl^- , Br^- , I^-

García *et al* (2006, 2007), Gravielle *et al* (2007)



$KI \approx K^{+} + I^{-}$

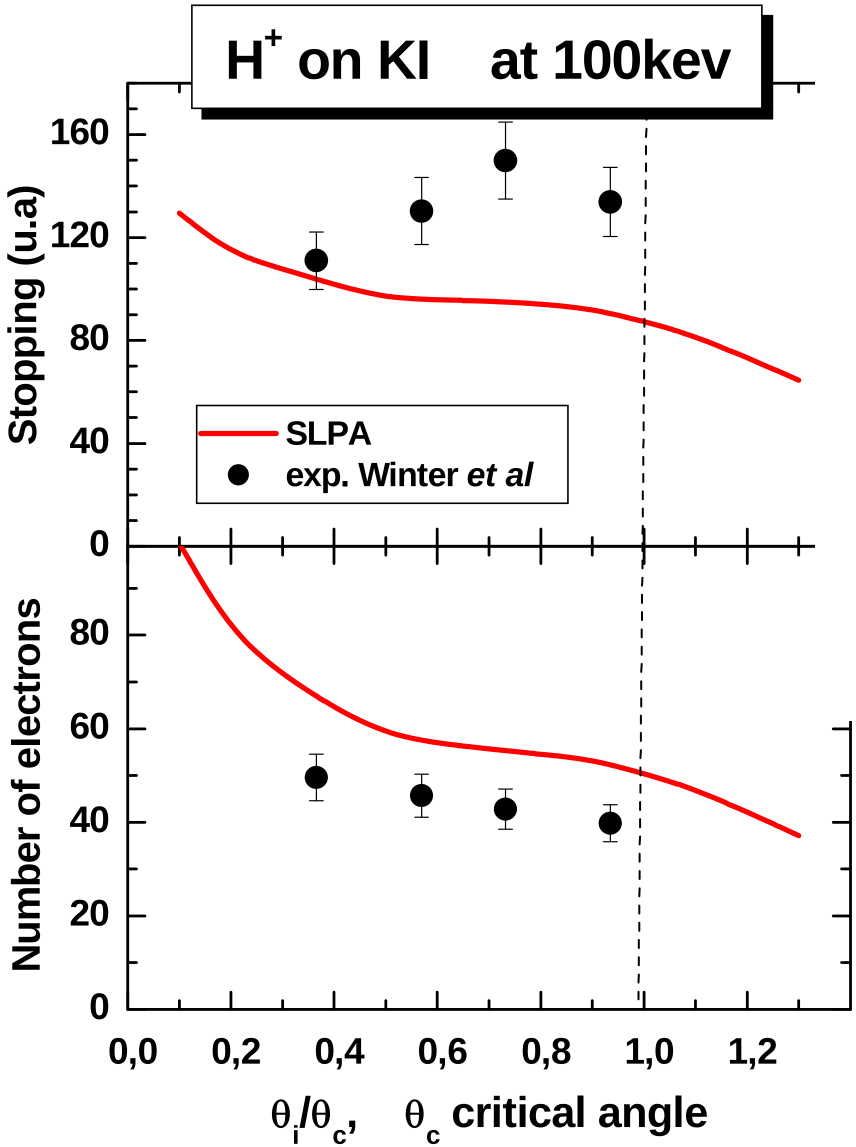
I^{-} 54 elects.

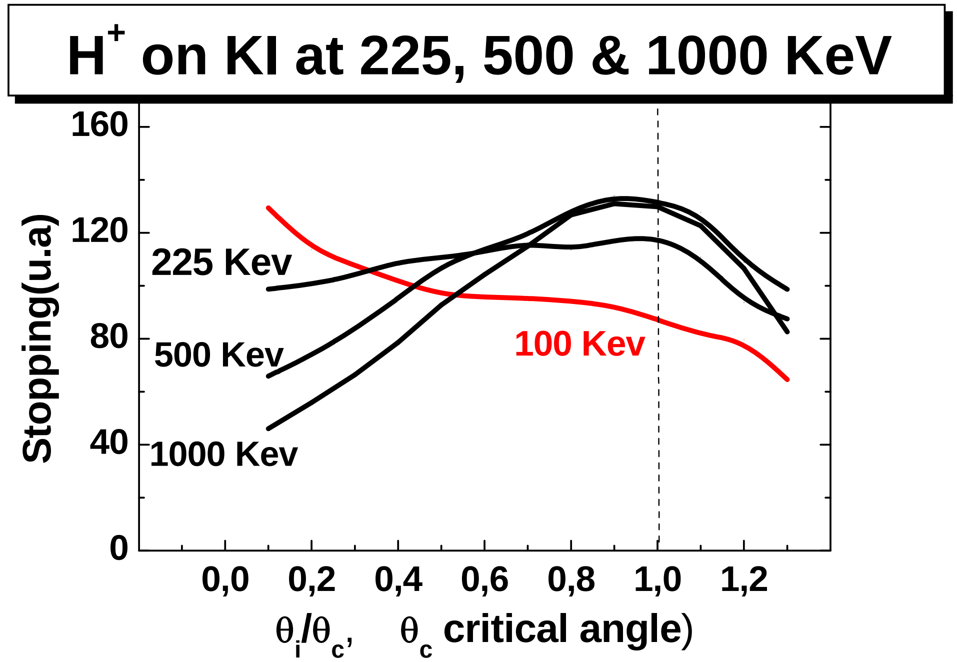
K^{+} 18 elects.

$< r >_{I^{-}\ 5p} = 2.7$

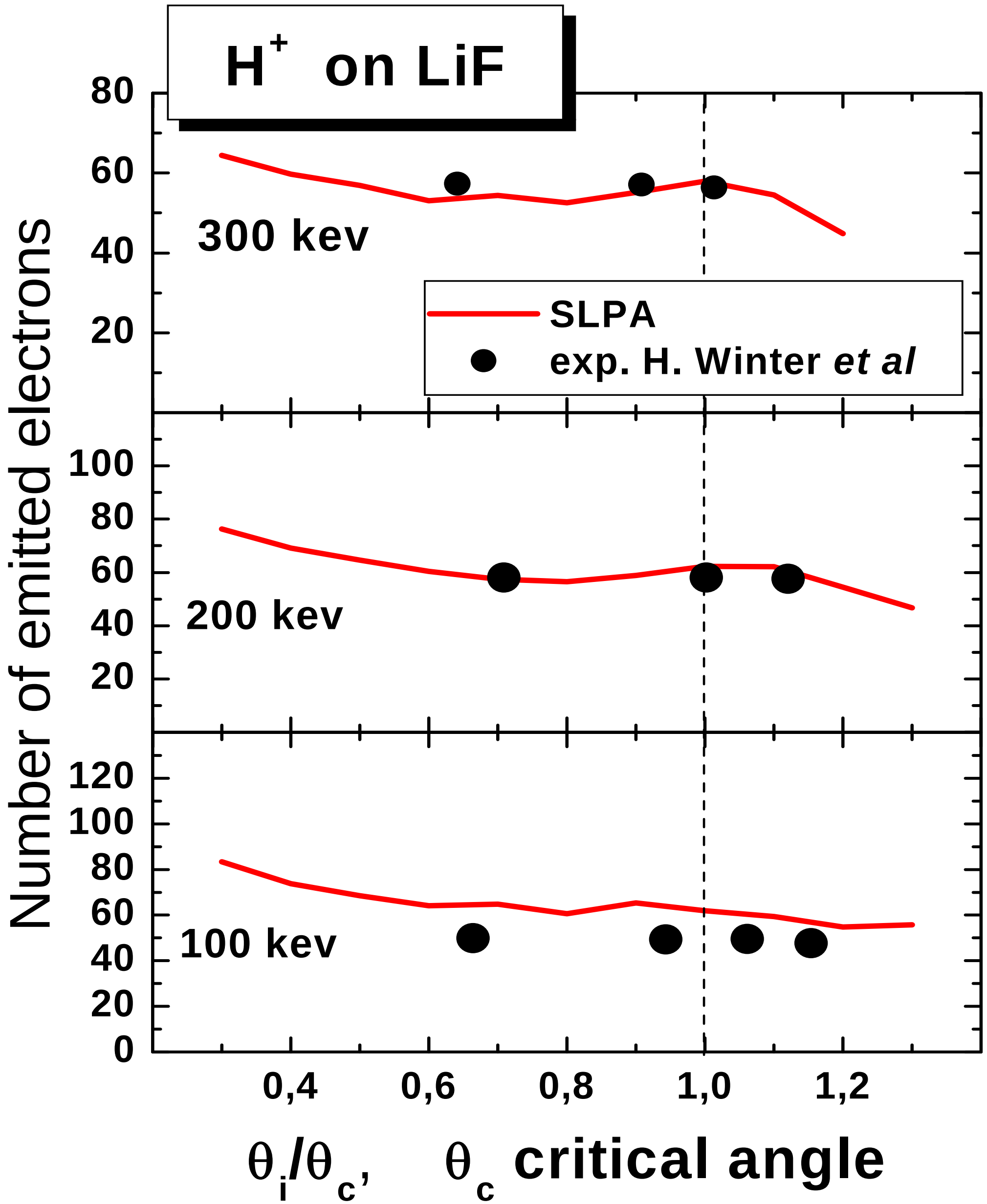
$< r >_{K^{+}\ 3p} = 1.5$

$\approx$ 1000 collisions





E (Kev)	θ_C (deg.)
100	1.23
225	0.84
500	0.57
1000	0.41



$LiF \approx Li^{+} + F^{-}$

F^{-} 10 elects.

Li^{+} 2 elects.

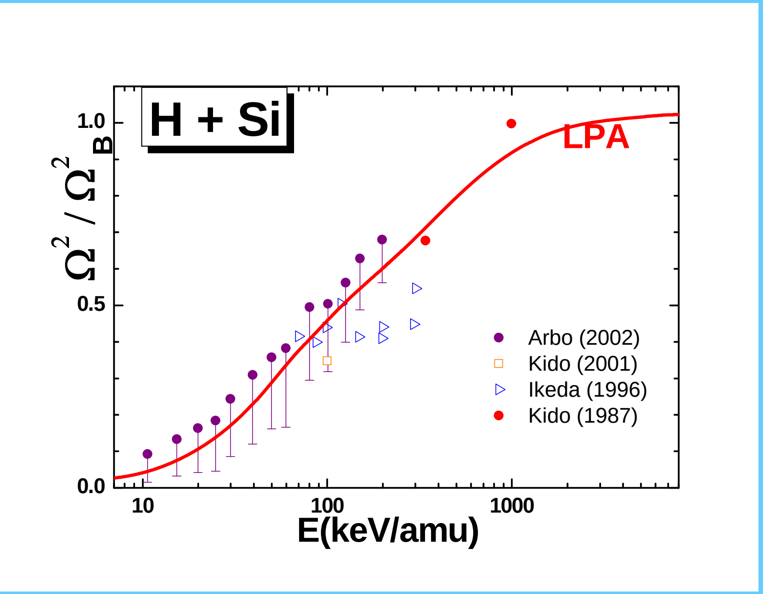
$< r >_{F^{-}\ 2p} = 1.25$

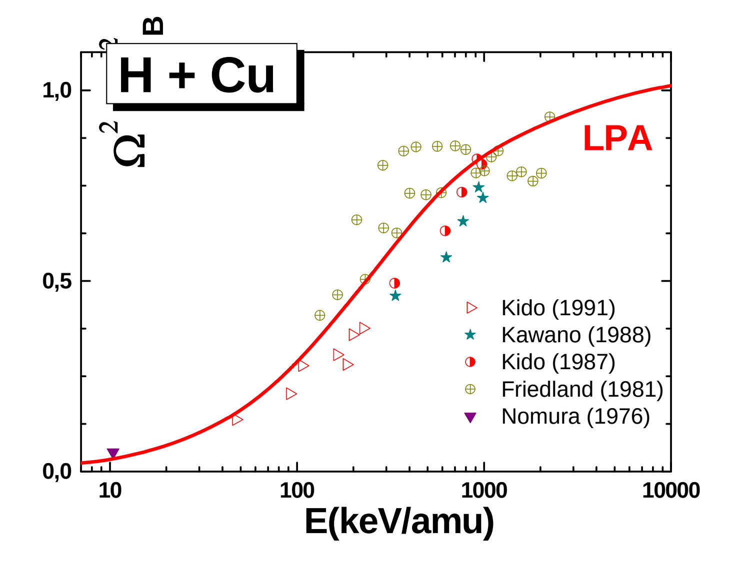
$< r >_{K^{+}\ 3p} = 0.44.$

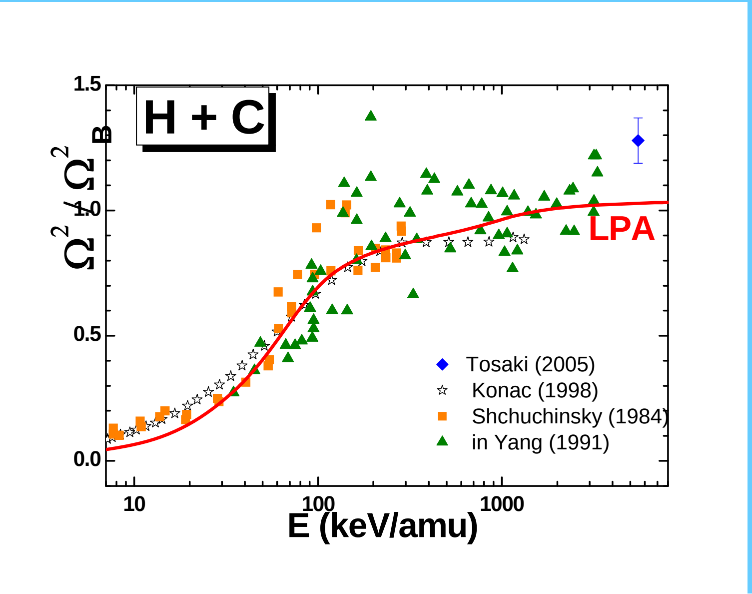
E (Kev)	θ_C (deg.)
100	0.84
225	0.60
500	0.42
1000	0.31

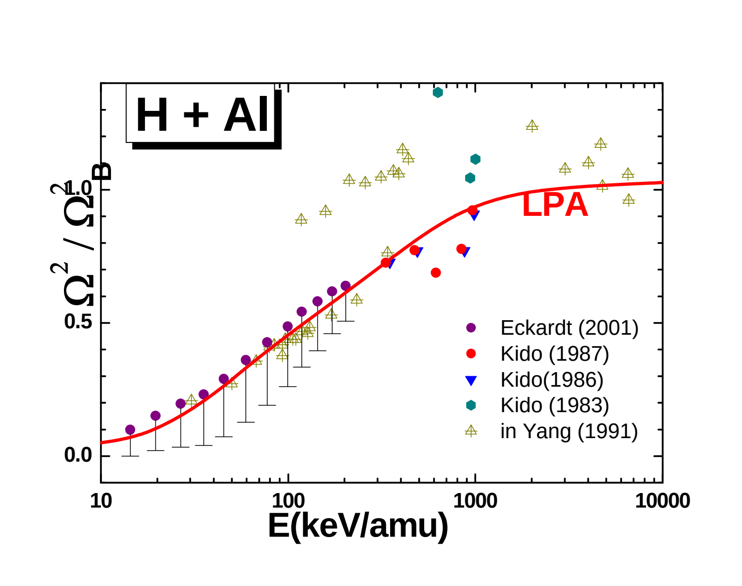
Straggling

$$\Omega^2 = \int_0^\infty d\omega\, \omega^2\, W(\omega), \qquad \Omega_B^2 = 4\pi N_e$$



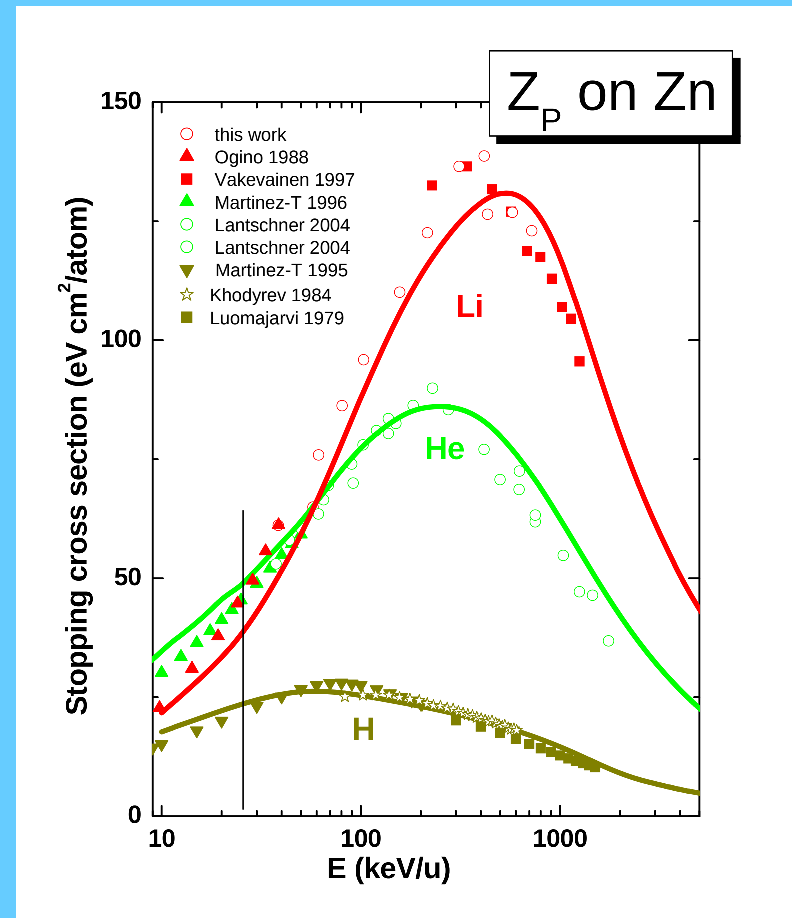


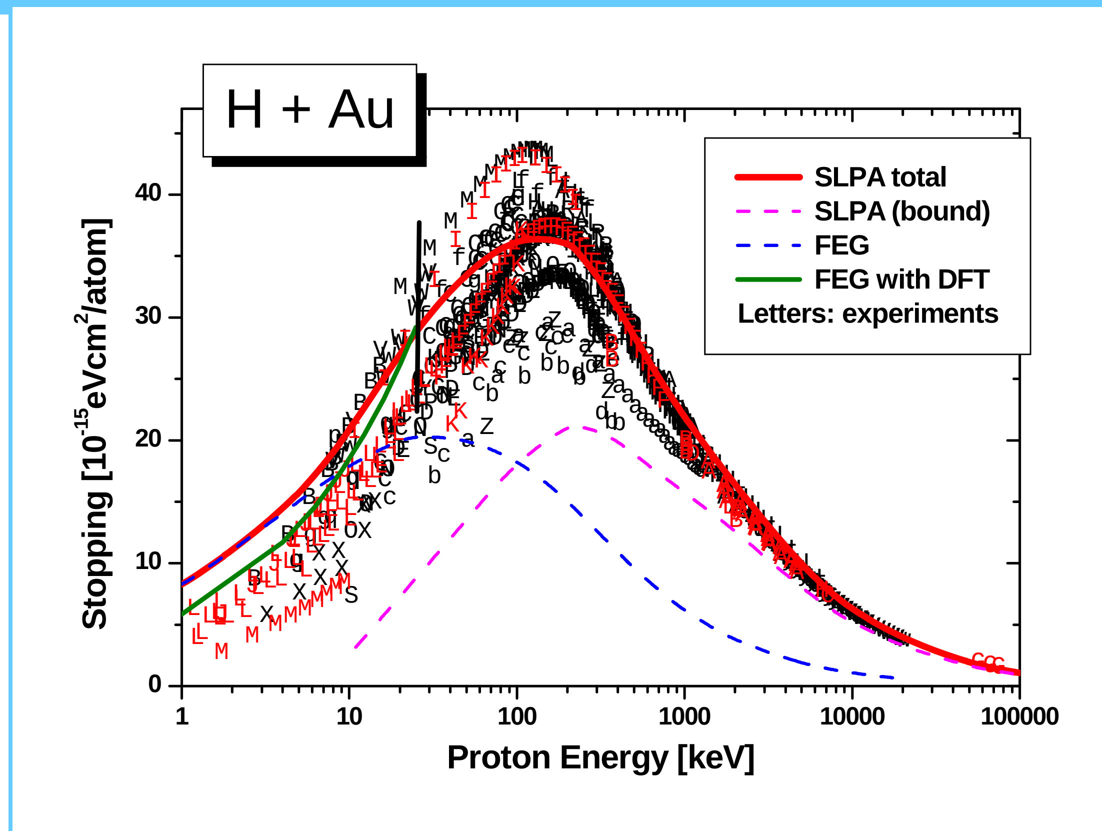




Stopping

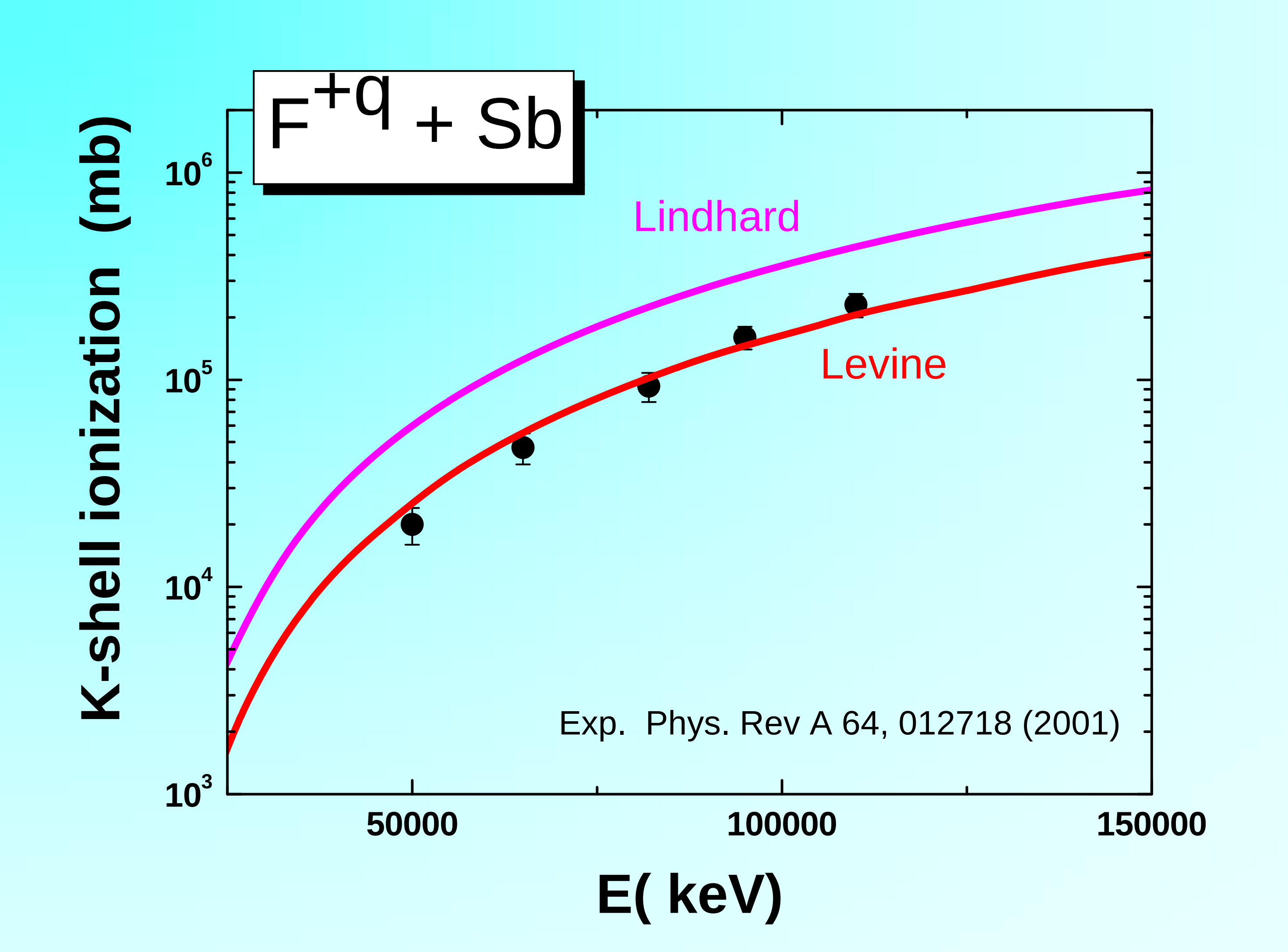
$$S = dE/dl = \int_{\varpi_g = \varepsilon_{nl}}^{\infty} d\omega\ \omega^{1}\ W(\omega(\omega$$





X-section

$$\sigma_{nl} = \int_{\omega_g = \varepsilon_{nl}}^{\infty} d\omega \ \omega^0 \ W_{nl}(\omega), \ \ /\text{atom}$$



Multiple Ionization

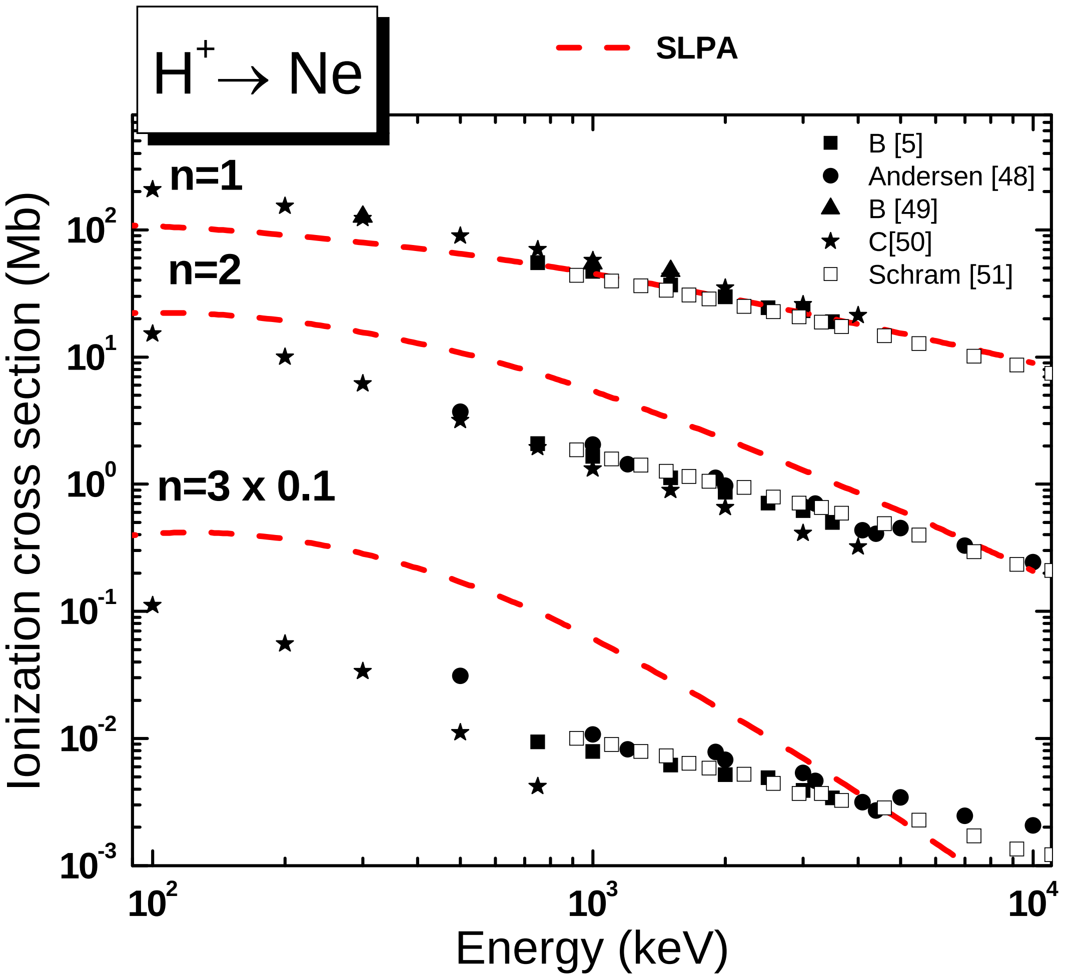
$$P_{nl}(\vec{b}) = \int_{-\infty}^{\infty} dz \int_{0}^{\infty} d\omega \int_{\omega/v}^{\infty} dq\ W_{nl}(q,\omega,z,b), \quad nl = \text{shell}$$

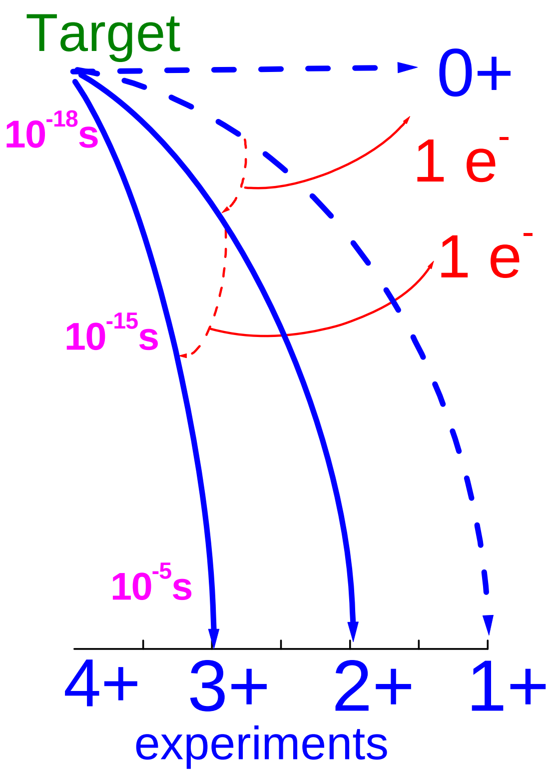
$$P(\vec{b}) = \sum_{nl} P_{nl}(\vec{b})$$ Differential probability

$$P_N(\vec{b}) = \frac{1}{N!} P^N(\vec{b}) \exp\left[-P(\vec{b})\right],$$ Poisson dist.

$$\sum_N P_N(\vec{b}) = 1\ ,$$ Normalization

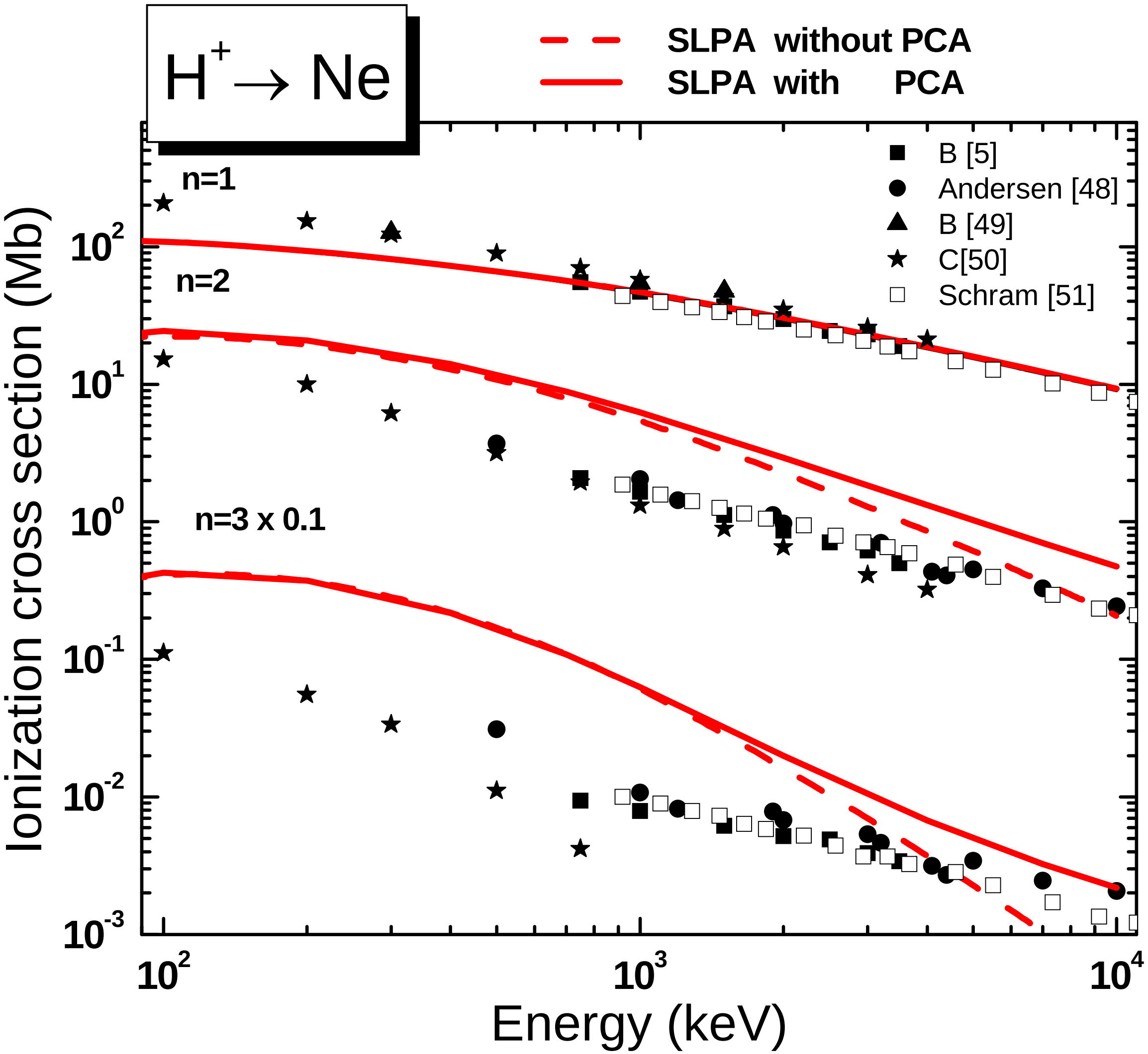
$$\sigma_N = \int d\vec{b}\ P_N(\vec{b}),$$ Xsection for N – ionization





Experimental ratio

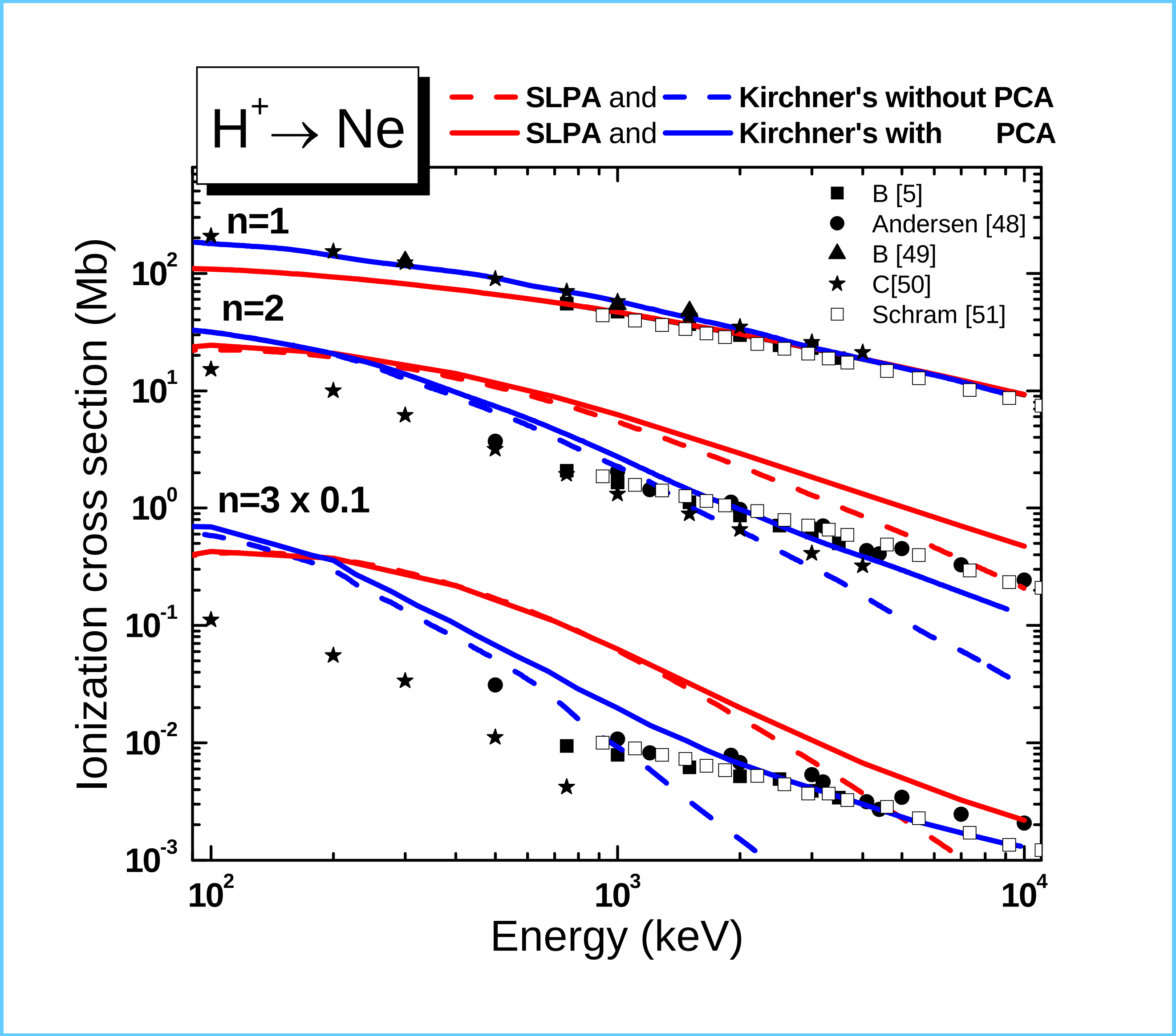
Morgan [21] (1997)



Experimental ratio

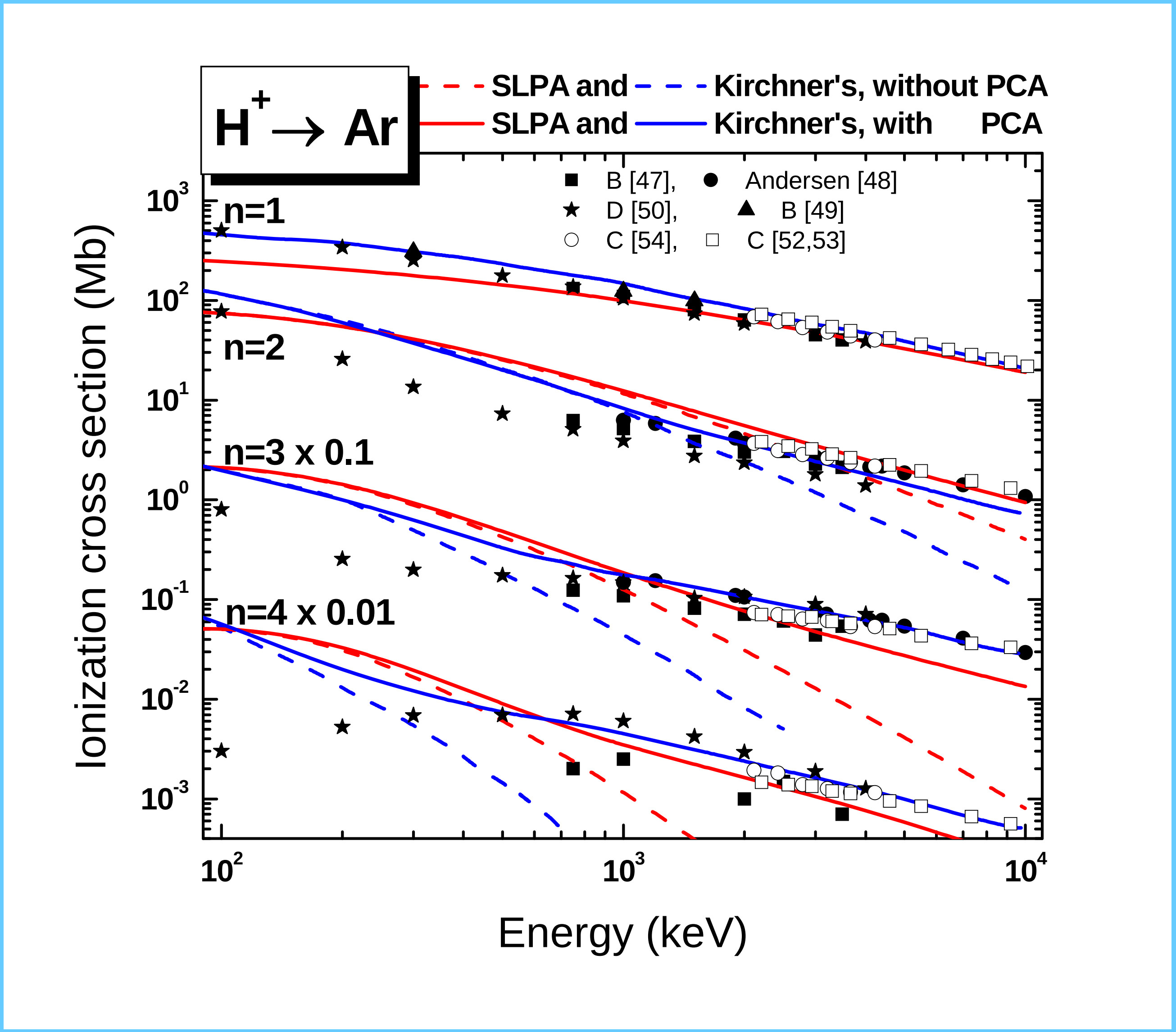
Morgan [21] (1997)

Ne	1s
F(nl,1+)	1.5%
F(nl,2+)	93.5
F(nl,3+)	4.8
F(nl,4+)	0.3



Experimetal ratios

Morgan [21] (1997)

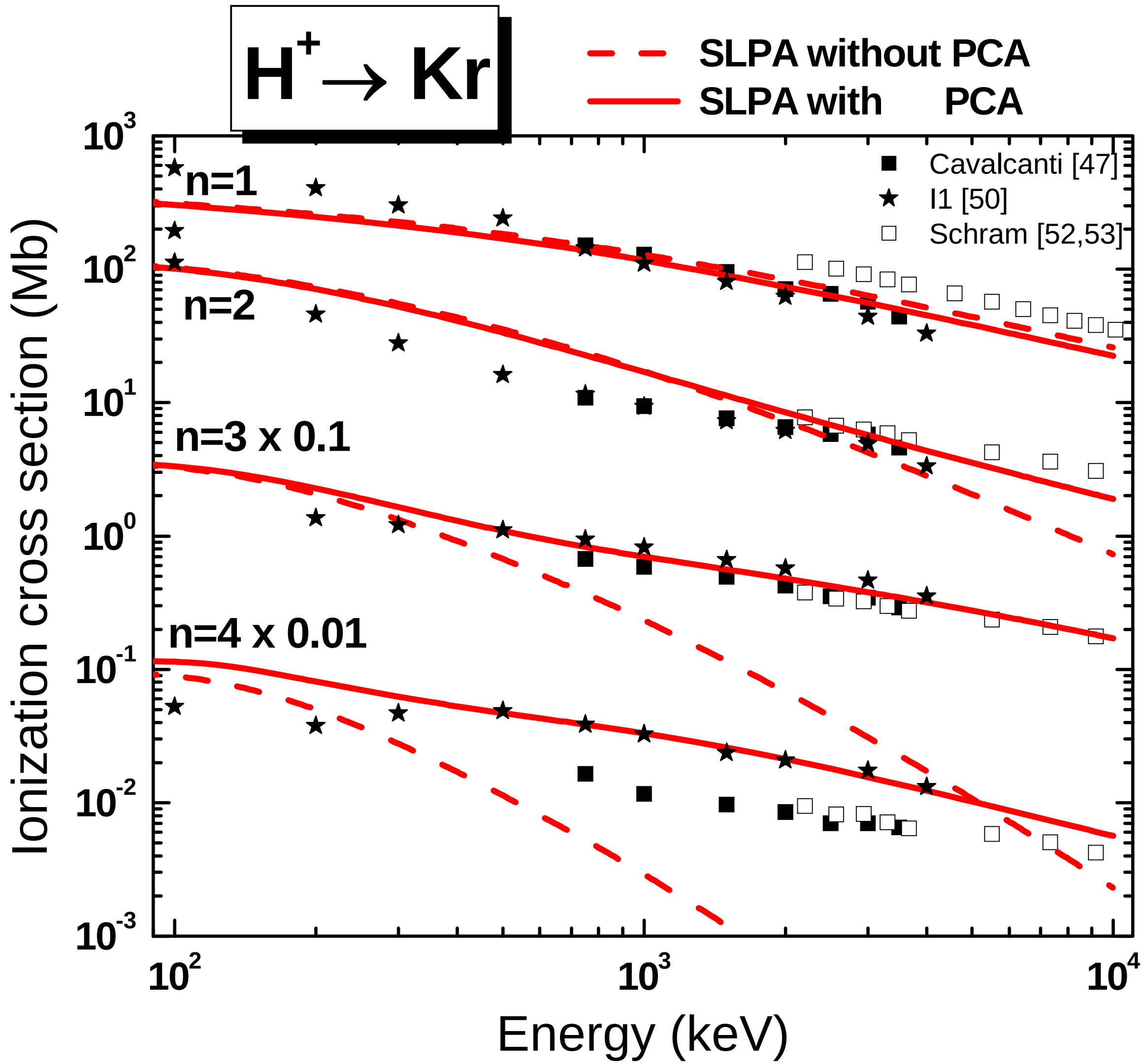


Experimental ratios

Carlson [45] (1966)

Brünken [23] (2002)

Ar	1s	2s	2p
F(nl,1+)	0.7	0.	0.5%
F(nl,2+)	10.5	1.	86.2
F(nl,3+)	7.8	89.	13.0
F(nl,4+)	42.7	10.	0.3



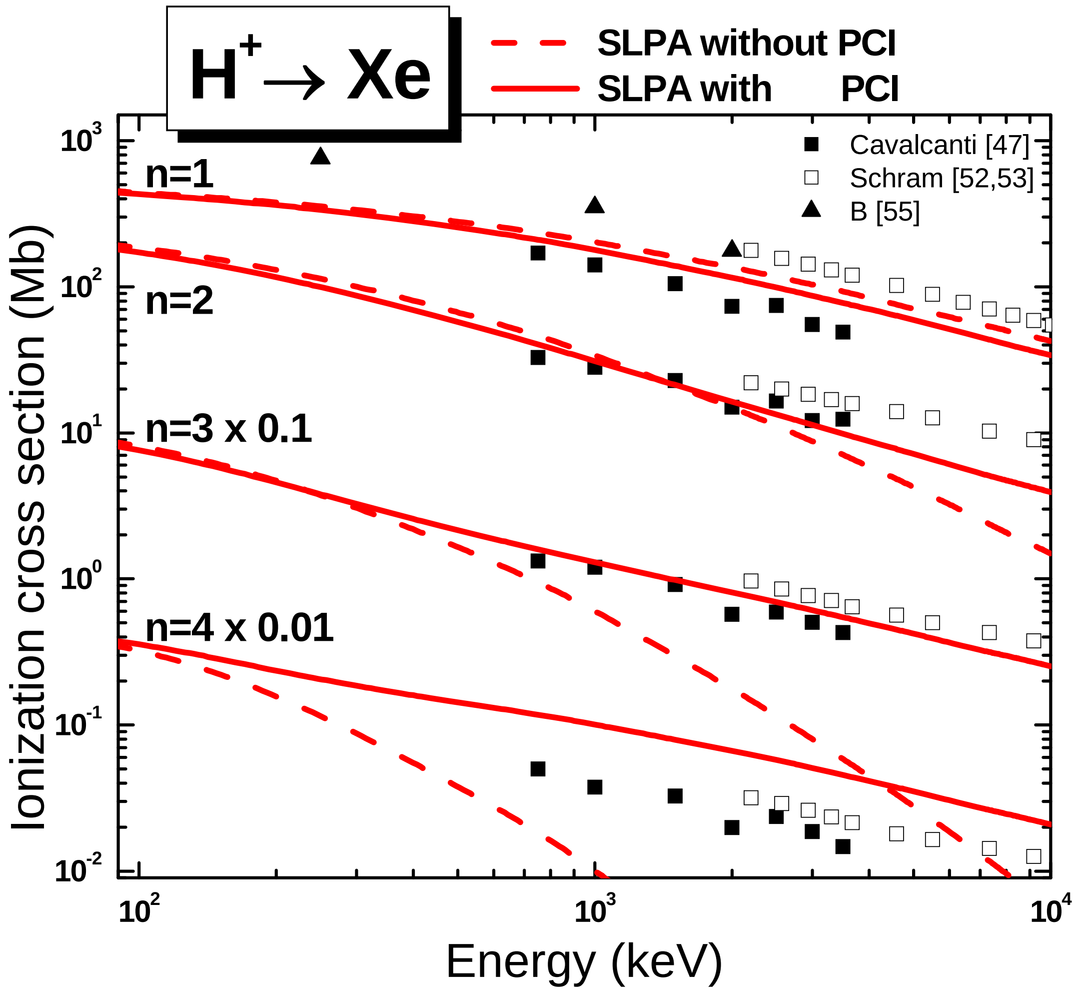
Experimental ratios

Carlson [45] (1966)

Armen [22] (2004)

Tamenori [24] (2004)

Kr	1s	2s	2p	3s	3p	3d
F(nl,1+)	1.	0.3	0.	0.	0.	2.%
F(nl,2+)	1.5	0.1	0.8	13.	3.5	56.
F(nl,3+)	6.	0.3	2.3	42.	58.6	38.
F(nl,4+)	17.	1.	31.	30.	32.6	3.



Experimental ratios

Carlson [45] (1966)

Saito [26] (1992)

Tamenori [27] (2004)

Hayaishi [28] (2002)

Kämmerling [29] (1992)

Xe	3s	3p	3d	4p	4d	N-shell
F(nl,1+)	0	0	0	0	1	5%
F(nl,2+)	0	0	0.3	0	80	40
F(nl,3+)	0	0	4	66	19	28
F(nl,4+)	0	0	39	34	0	21

Resumé

<u>Advantages</u> of the SLPA:

1- e-e correlation to all order

2- Just the electron densities & binding energies.

Do not need the continuum. Good for DFT used in QCh.

3- Cartesian coordinates. Not needed central potential

4- Projectile classical trajectory selfconsistent (e impact)

<u>Disadvantages</u>

1- First order in the projectile charge

2- It is local

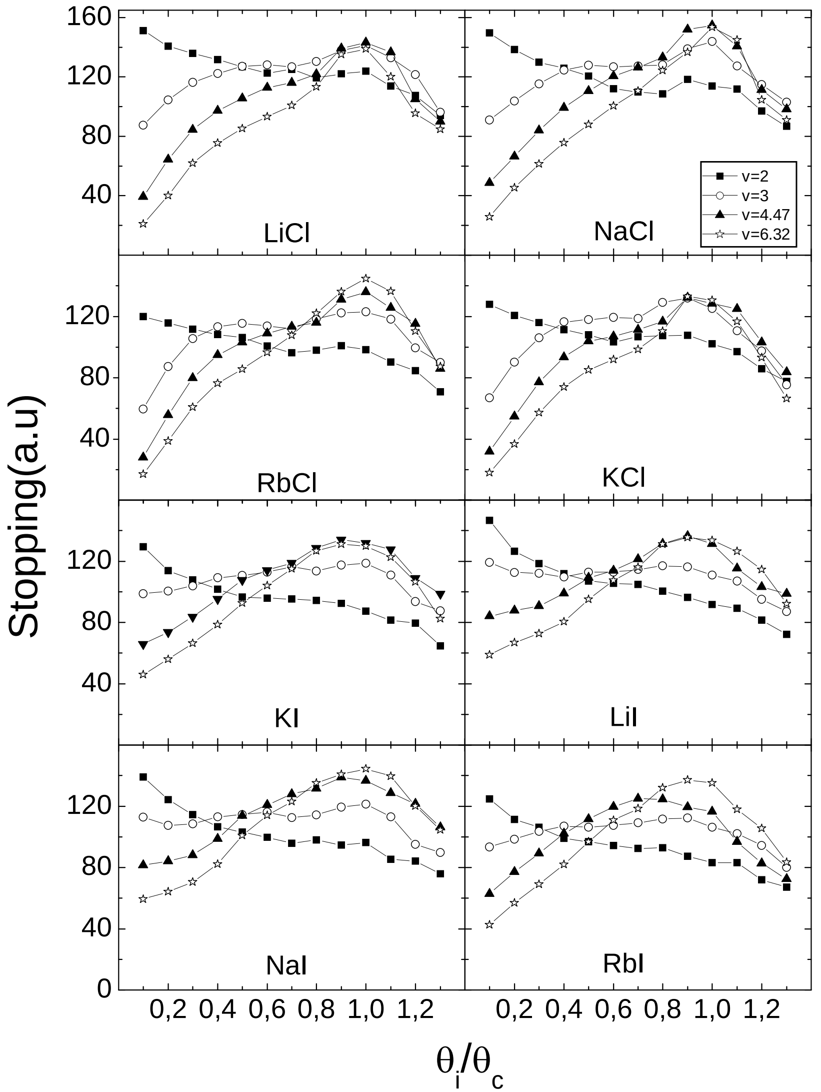
3- It is a model. No perturbative series to follow

Future Developmens

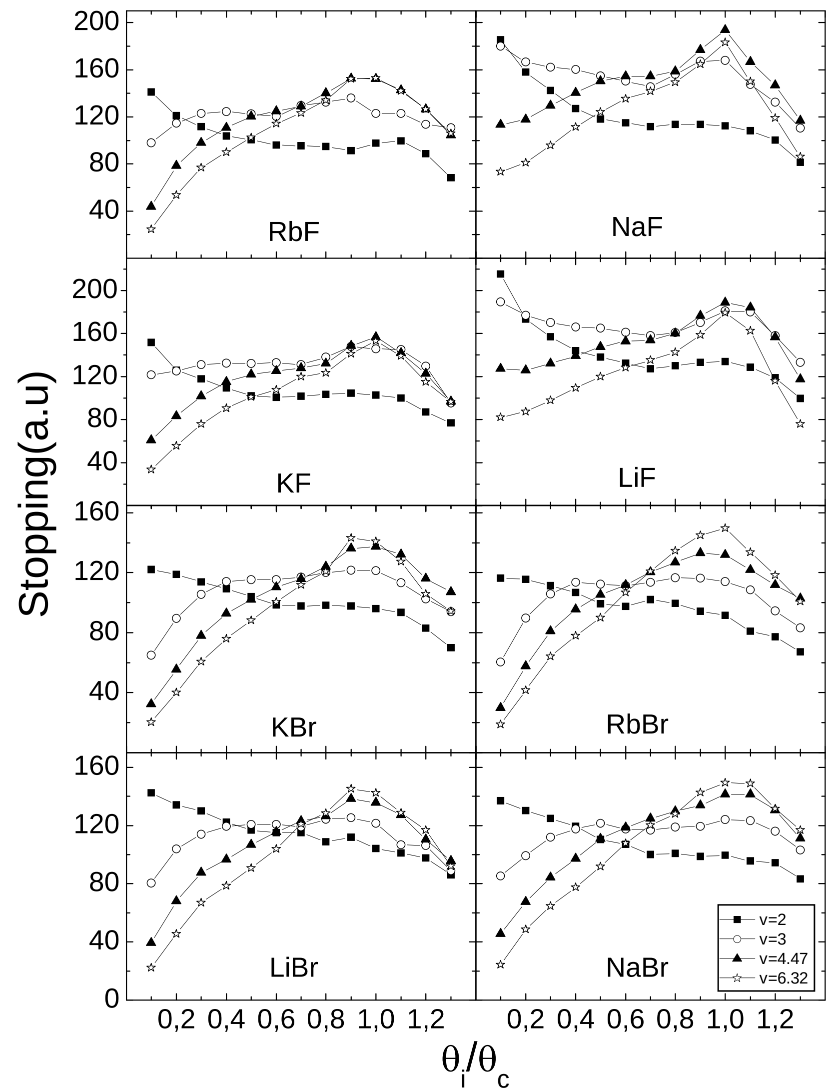
1- Heavy atoms f-shell , molecules & clusters

2- Atom-atom antiscreening (= collision of two FEG)

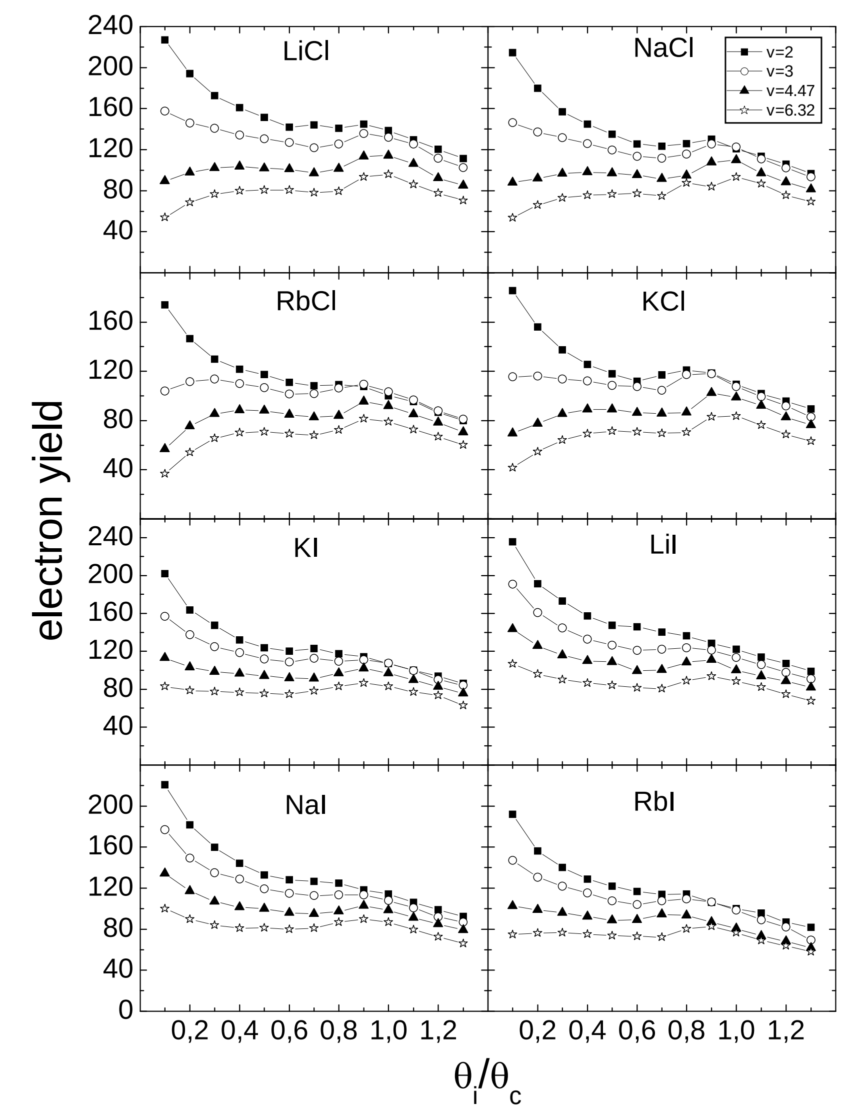
3- Improve the Local hypothesis by extending to momentum space. Intense activity in QCh

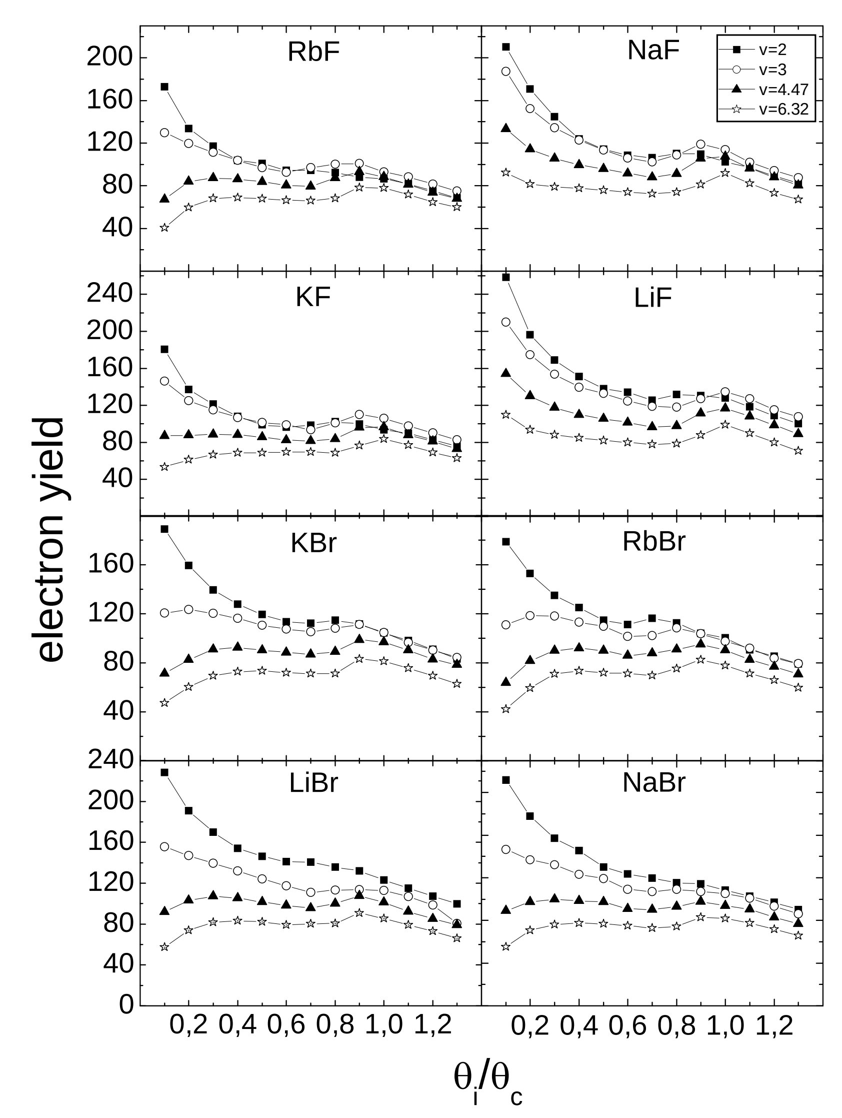


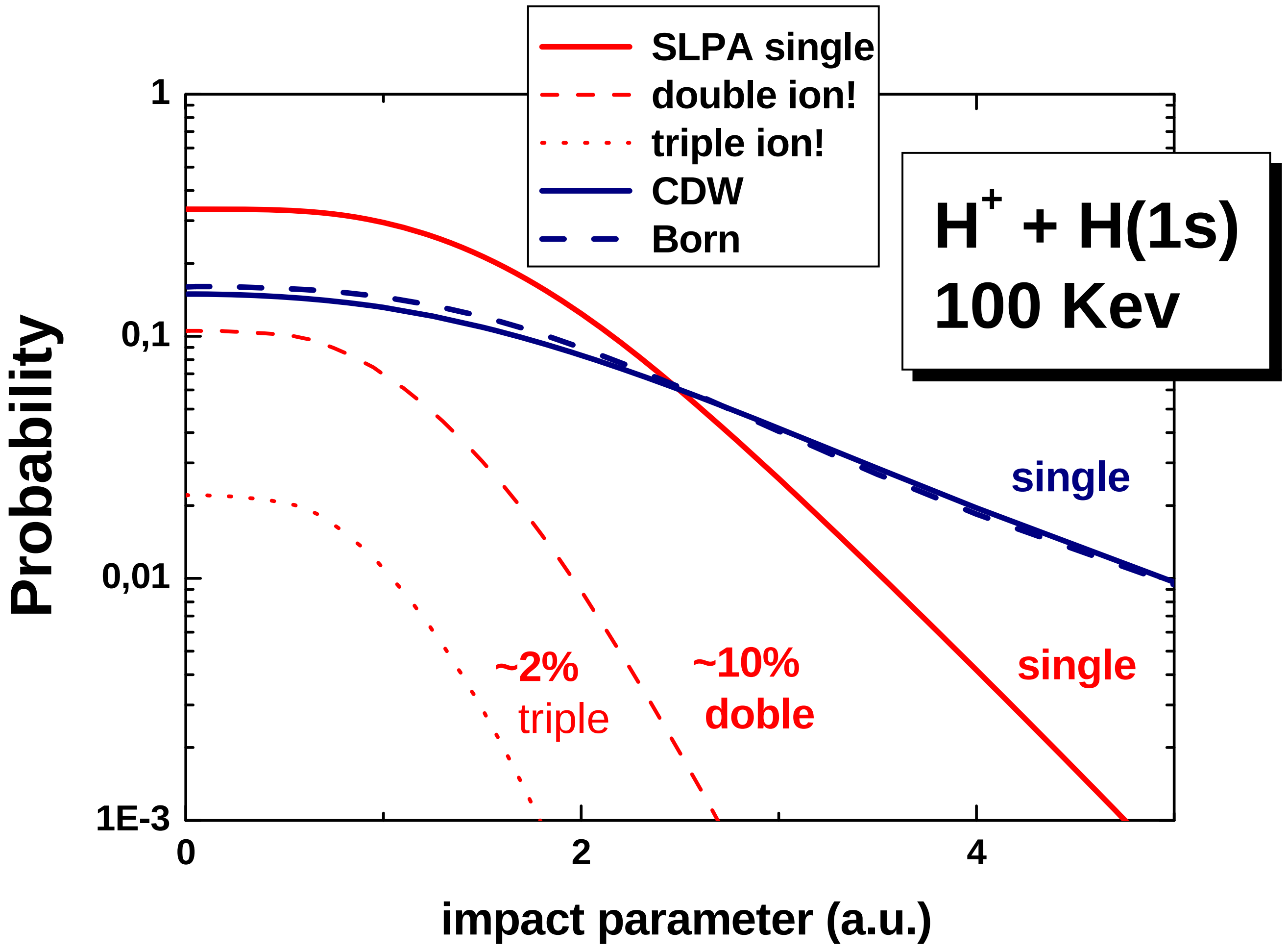
Stopping(a.u)
LiCl
NaCl
RbCl
KCl
KI
LiI
NaI
RbI
v=2
v=3
v=4.47
v=6.32
θi/θc



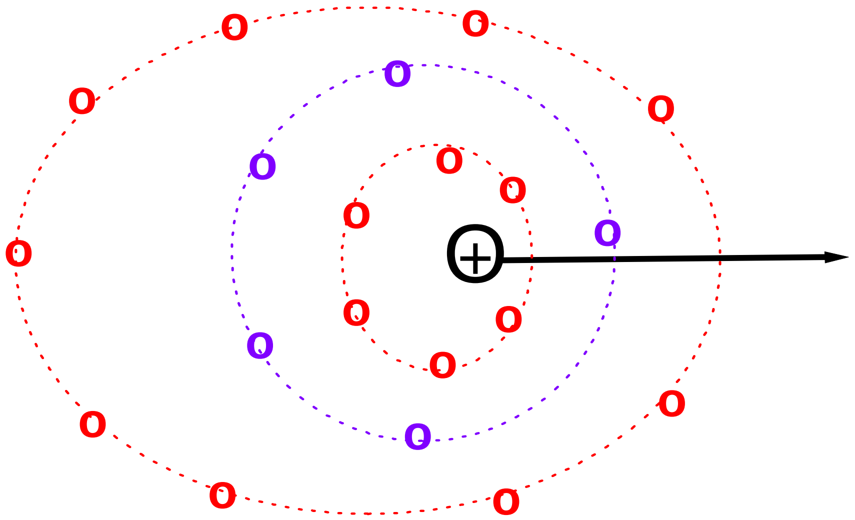
Stopping(a.u)
RbF
NaF
KF
LiF
KBr
RbBr
LiBr
NaBr
v=2
v=3
v=4.47
v=6.32
θi/θc


LiCl
NaCl
RbCl
KCl
KI
LiI
NaI
RbI
v=2
v=3
v=4.47
v=6.32
electron yield
θi/θc

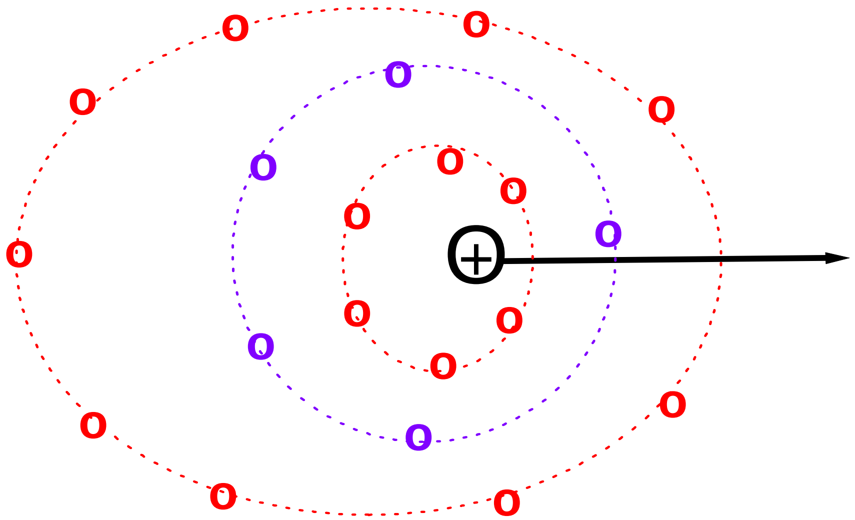

RbF
NaF
KF
LiF
KBr
RbBr
LiBr
NaBr
v=2
v=3
v=4.47
v=6.32
electron yield
θi/θc

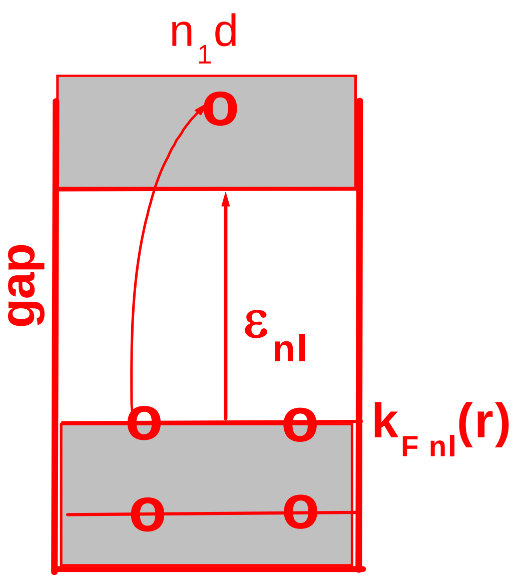

SLPA single
double ion!
triple ion!
CDW
Born
H^+ + H(1s)
100 Kev
1
0,1
0,01
1E-3
Probability
0
2
4
impact parameter (a.u.)
single
single
~2%
triple
~10%
doble

Independent Shell approximation - SLPA

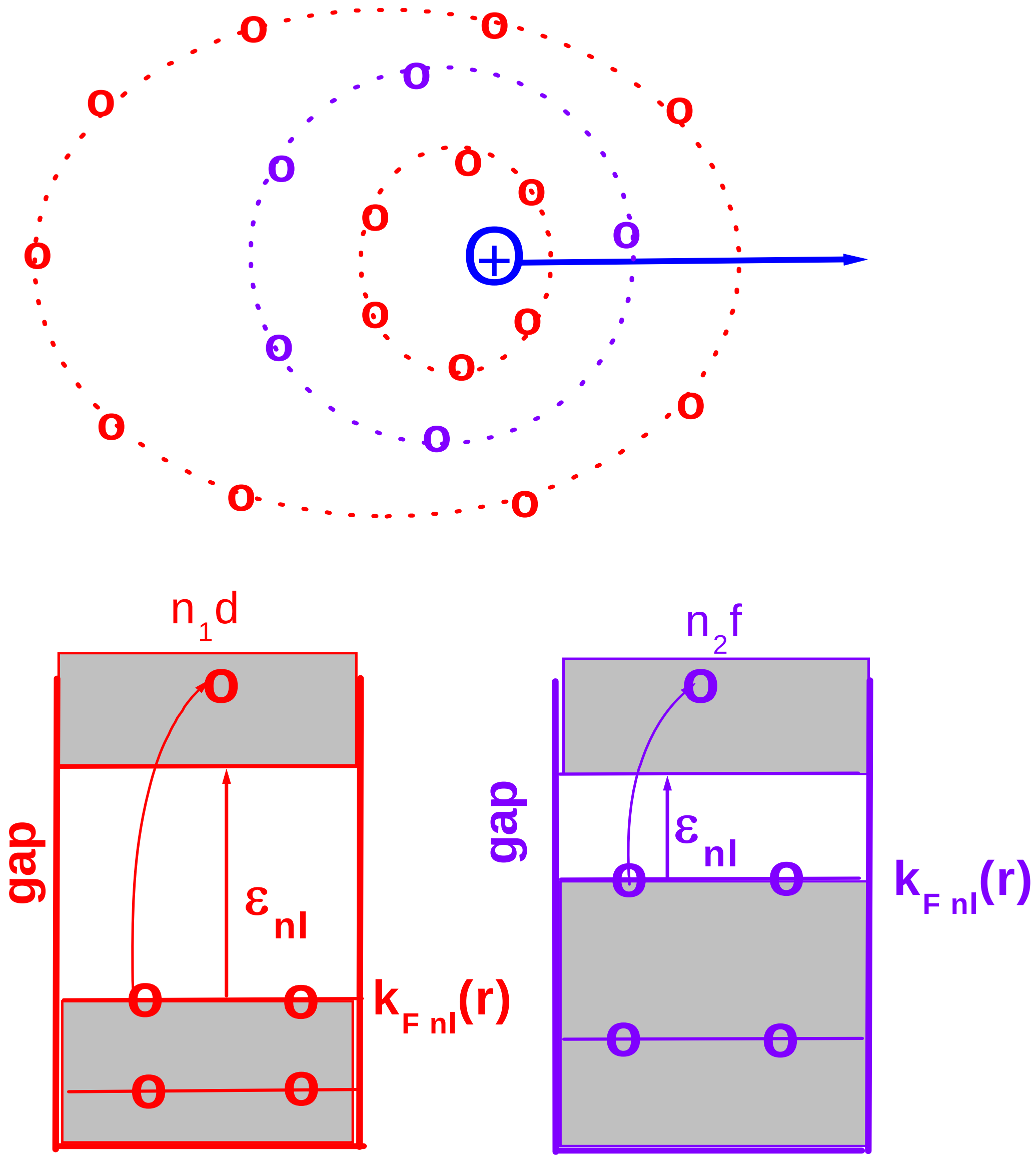


Independent Shell approximation - SLPA





Independent Shell approximation - SLPA



Boltzman (transport) Equation

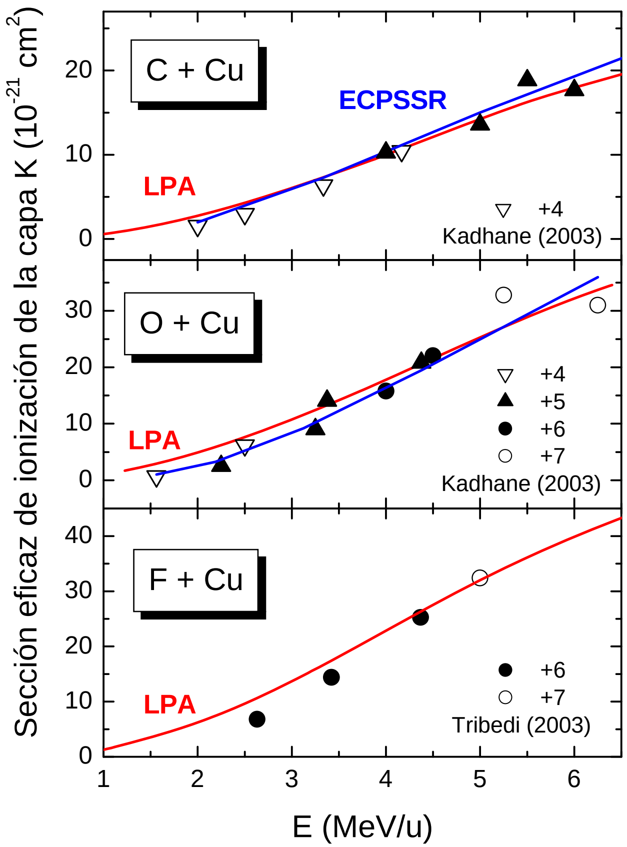
$$\frac{\partial g(E,z,b)}{\partial z} = \int_0^{E_0} d\omega \;\; W(\omega,z,b)\left[g(E+\omega,z,b) - g(E,z,b)\right]$$

$g(E,z,b) =$ **Projectile energy distribution function**

$$W(\omega,z,b) = \textbf{Kernel} = \int_{\omega/v}^{\infty} dq\, W(\omega,q,z,b)$$

$$W(\omega,q,z,b) = \frac{2Z_P^2}{\pi v^2}\frac{1}{q}\,\mathrm{Im}\left[\frac{1}{\varepsilon(q,\omega,k_F(\delta(\vec{r}))}\right]$$

Lencinas(90), Archubi (07)


C + Cu
ECPSSR
LPA
+4
Kadhane (2003)
O + Cu
LPA
+4
+5
+6
+7
Kadhane (2003)
F + Cu
LPA
+6
+7
Tribedi (2003)
Sección eficaz de ionización de la capa K (10^{-21} cm^2)
E (MeV/u)

charged ions in photoionization experiments. This ratios $F_{nl,i}$ express how the direct single ionization of a certain nl shell contributes to ion formation of charge $+i$, so that $\sum_i F_{nl,i} = 1$. Including these ratios in (14) we obtain

$$p(b) = \sum_{nl} p_{nl}(b) \times 1 = \sum_{nl} p_{nl}(b) \times \sum_i F_{nl,i} = \sum_{i=1}^{Z_T} \mathcal{P}_i(b) \tag{16}$$

with

$$\mathcal{P}_i(b) = \sum_{nl} p_{nl}(b) F_{nl,i} \tag{17}$$

being the probability of a direct single ionization (of any shell nl) followed by post-collisional emission of $i-1$ electrons. Replacing (16) in (10) and rearranging terms so

as to put together those that contribute to the same number of final emitted electrons, we can express ionization probabilities including post-collisional emission as $P_N^{post}(b)$

$$P_1^{post} = e^{-p(b)} \mathcal{P}_1, \tag{18a}$$

$$P_2^{post} = e^{-p(b)} \left[\mathcal{P}_2 + \frac{\mathcal{P}_1^2}{2!} \right], \tag{18b}$$

$$P_3^{post} = e^{-p(b)} \left[\mathcal{P}_3 + \frac{2\mathcal{P}_1 \mathcal{P}_2}{2!} + \frac{\mathcal{P}_1^3}{3!} \right], \tag{18c}$$

$$P_4^{post} = e^{-p(b)} \left[\mathcal{P}_4 + \frac{2\mathcal{P}_1 \mathcal{P}_3}{2!} + \frac{\mathcal{P}_2^2}{2!} + \frac{3\mathcal{P}_1^2 \mathcal{P}_2}{3!} + \frac{\mathcal{P}_1^4}{4!} \right], \tag{18d}$$

where we have shortened $\mathcal{P}_N(b)$ and $P_N^{post}(b)$ by $\mathcal{P}_N$ and P_N^{post}. Each expression P_N^{post} includes the term $e^{-p(b)} \mathcal{P}_1^N / N!$ that considers all the combination of direct ionization probabilities of N electrons of different shells, and the term $e^{-p(b)} \mathcal{P}_N$ that corresponds to a single ionization followed by the emission of $N-1$ electrons via Auger