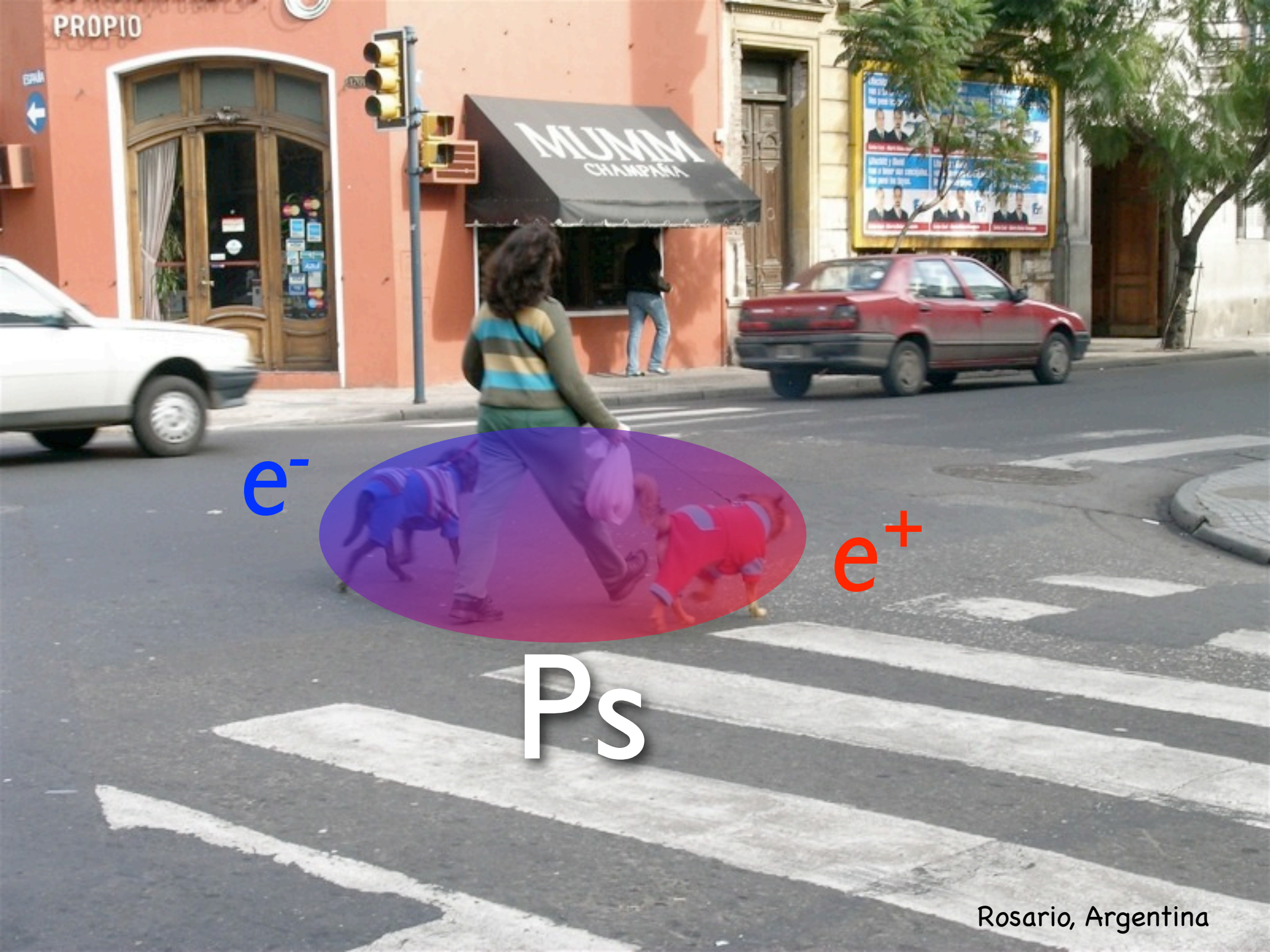
Rosario, Argentina


PROPIO
MUMM
CHAMPAÑA
e^-
e^+
Ps
Rosario, Argentina

Queen's University Belfast

Low-energy positron interactions with atoms and molecules

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Department of Applied Mathematics and Theoretical Physics
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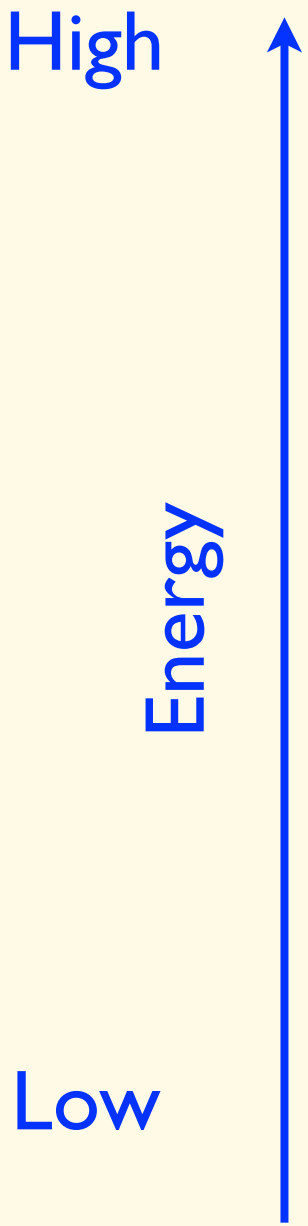
Positron collisions



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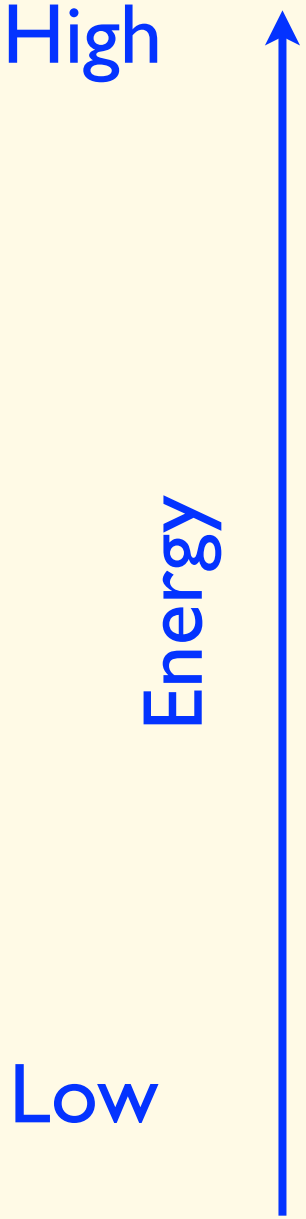
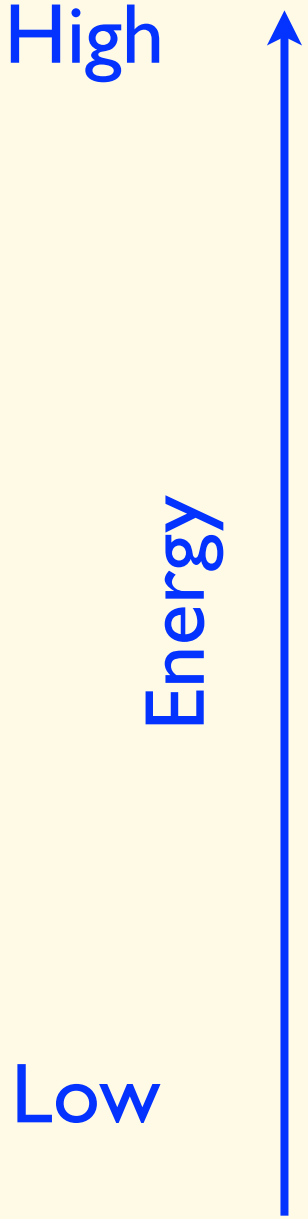


$$e^+ + A \longrightarrow A^+ + e^+ + e^-$$

Positron collisions



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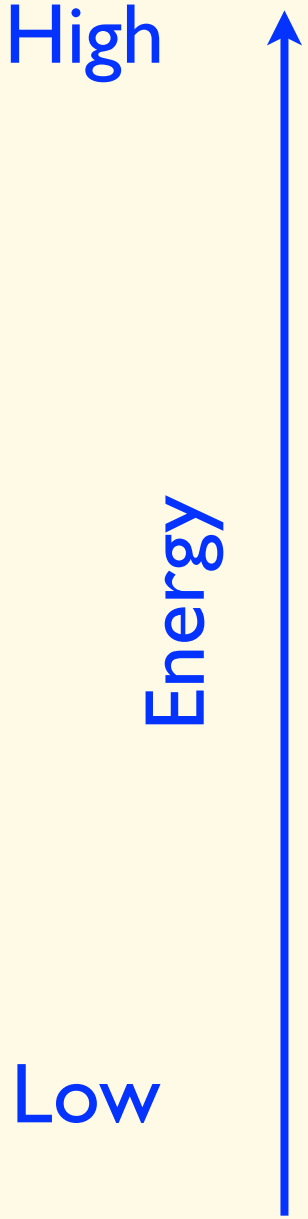
$$e^+ + A \longrightarrow A^* + e^+$$

Positron collisions



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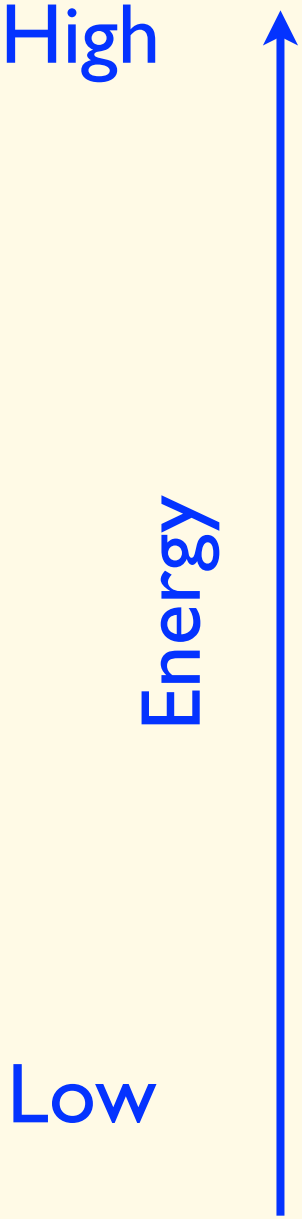
$$e^+ + A \longrightarrow A^* + e^+$$

$$e^+ + A \longrightarrow A + \mathrm{Ps}$$

Positron collisions



$$e^+ + A \longrightarrow A^+ + e^+ + e^-$$

$$e^+ + A \longrightarrow A^* + e^+$$

$$e^+ + A \longrightarrow A + \mathrm{Ps} \quad \varepsilon > I - 6.8 \text{ eV}$$

Positron collisions

High

Energy

Low

$$e^+ + A \longrightarrow A^+ + e^+ + e^-$$

$$e^+ + A \longrightarrow A^* + e^+$$

$$e^+ + A \longrightarrow A + \mathrm{Ps} \quad \varepsilon > I - 6.8 \text{ eV}$$

$$e^+ + A \longrightarrow A + e^+ \qquad \text{elastic}$$

Positron collisions

High

Energy

Low

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Positron collisions

High

Energy

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Positron collisions

High

Energy

Low

Negative

$$e^+ + A \longrightarrow A^+ + e^+ + e^-$$

$$e^+ + A \longrightarrow A^* + e^+$$

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High

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Low

Negative

e^+A $\qquad$ e^+M $\qquad$ binding

Main points

- Low-energy positron interaction with atoms and molecules is attractive
- For mildly attractive targets this results in low-lying positron virtual levels
- Elastic scattering and annihilation are enhanced
- Positrons can form bound states with many neutral species
- For molecules positron binding gives rise to vibrational Feshbach resonances
- Vibrational Feshbach resonances can lead to very large annihilation rates
- Resonant annihilation is enhanced by intramolecular vibrational energy redistribution (a ubiquitous effect!)
- Observation of vibrational Feshbach resonances in annihilation allows measurement of positron binding energies for many molecules
- Larger molecules can possess multiple positron bound states

Positron theory milestones I

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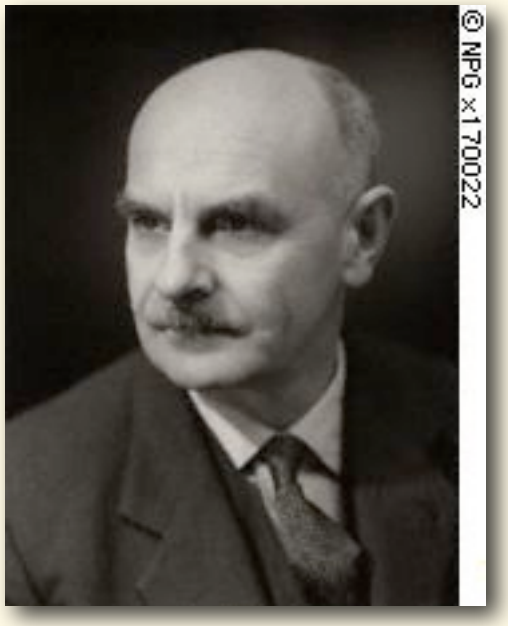

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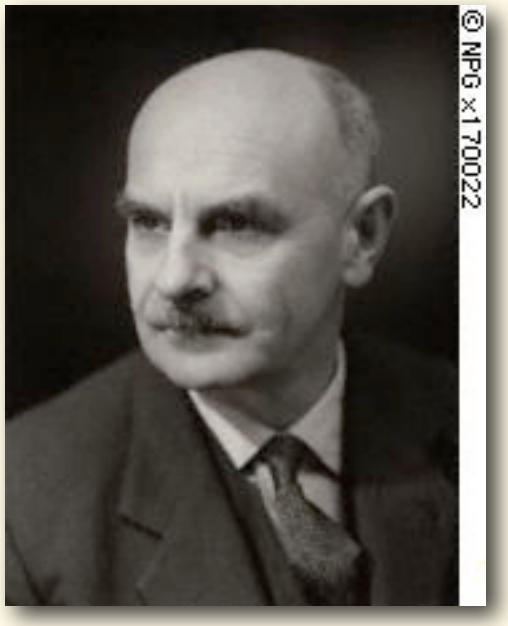

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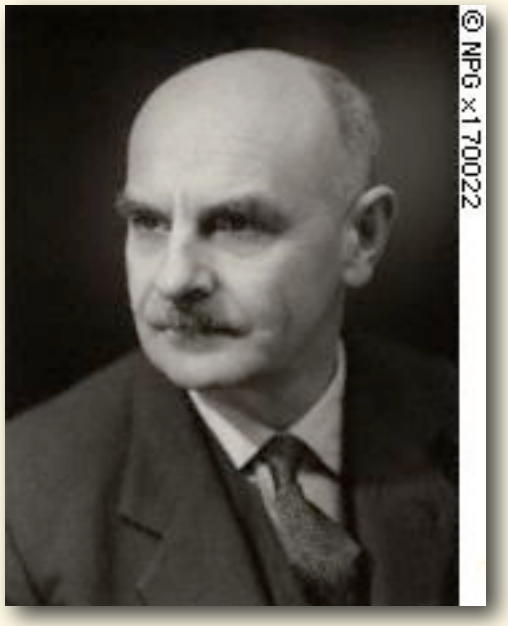

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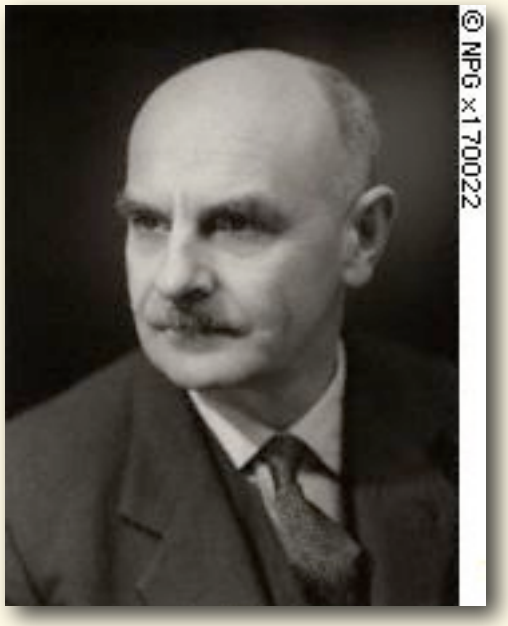

"... The annihilation studies [...] are completely mysterious at present, in almost all substances, and particularly for instance in xenon and krypton and methane and so on."

Round-table discussion on future directions in positron-gas research
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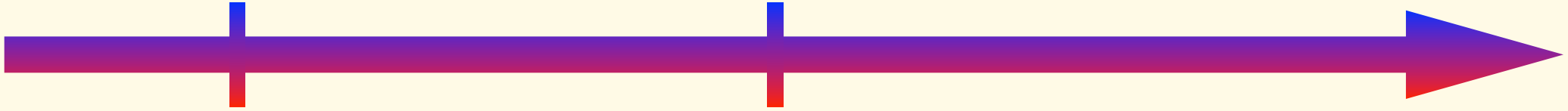

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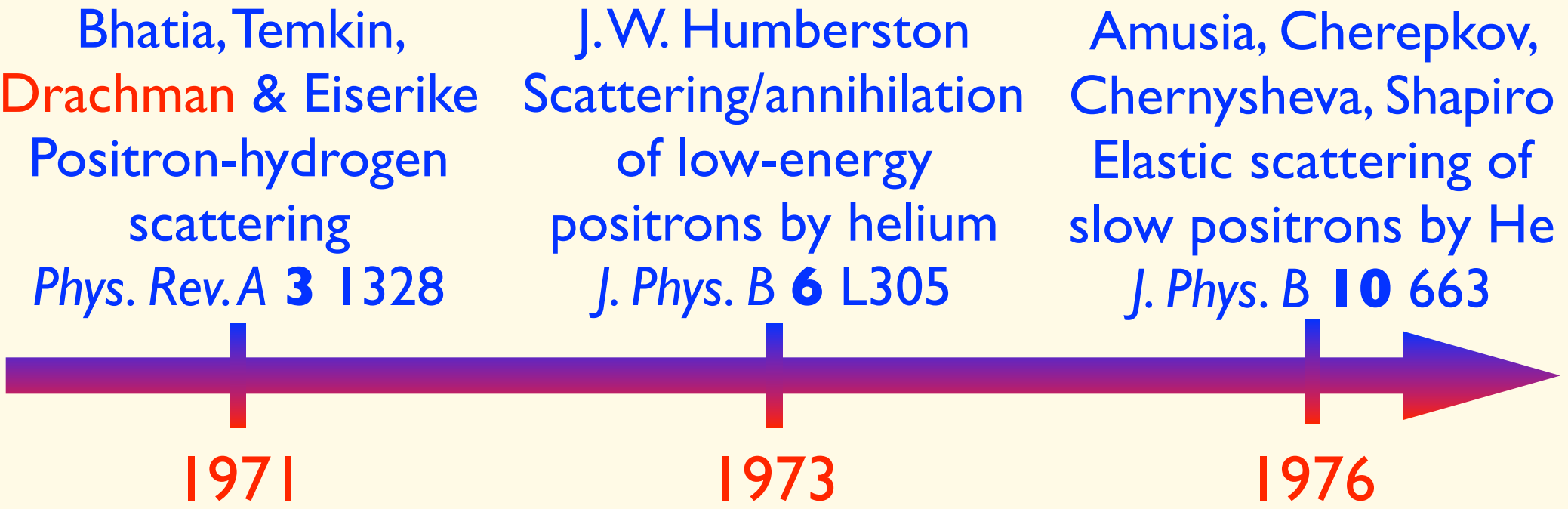

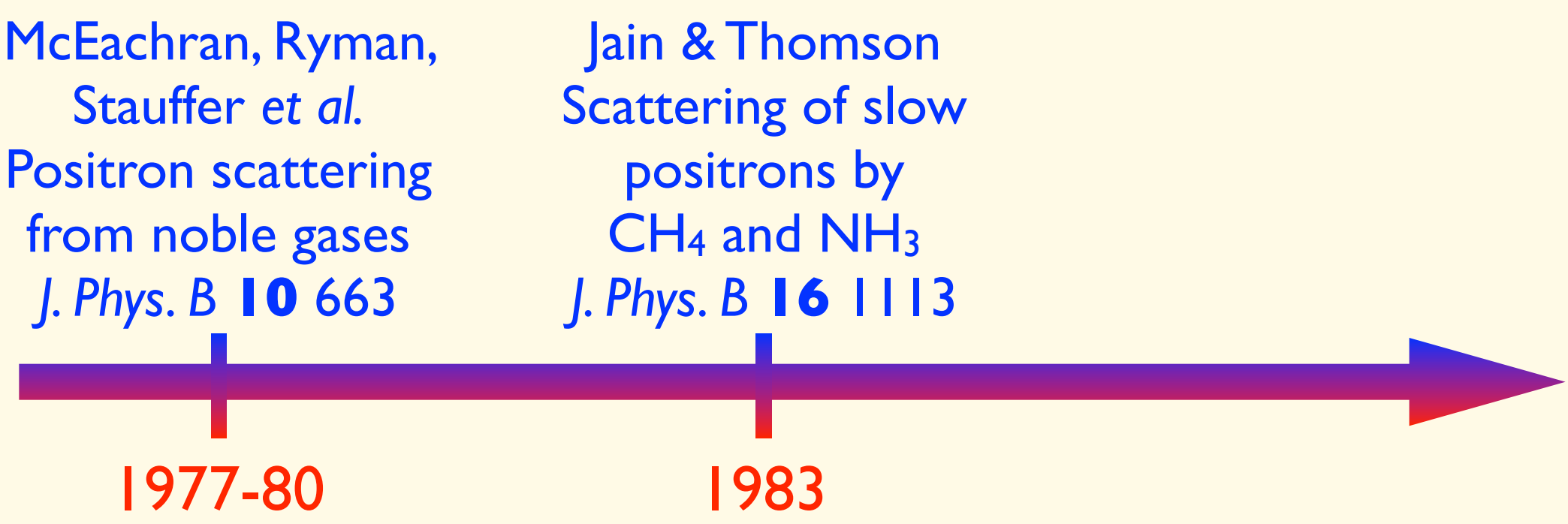

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Jain & Thomson
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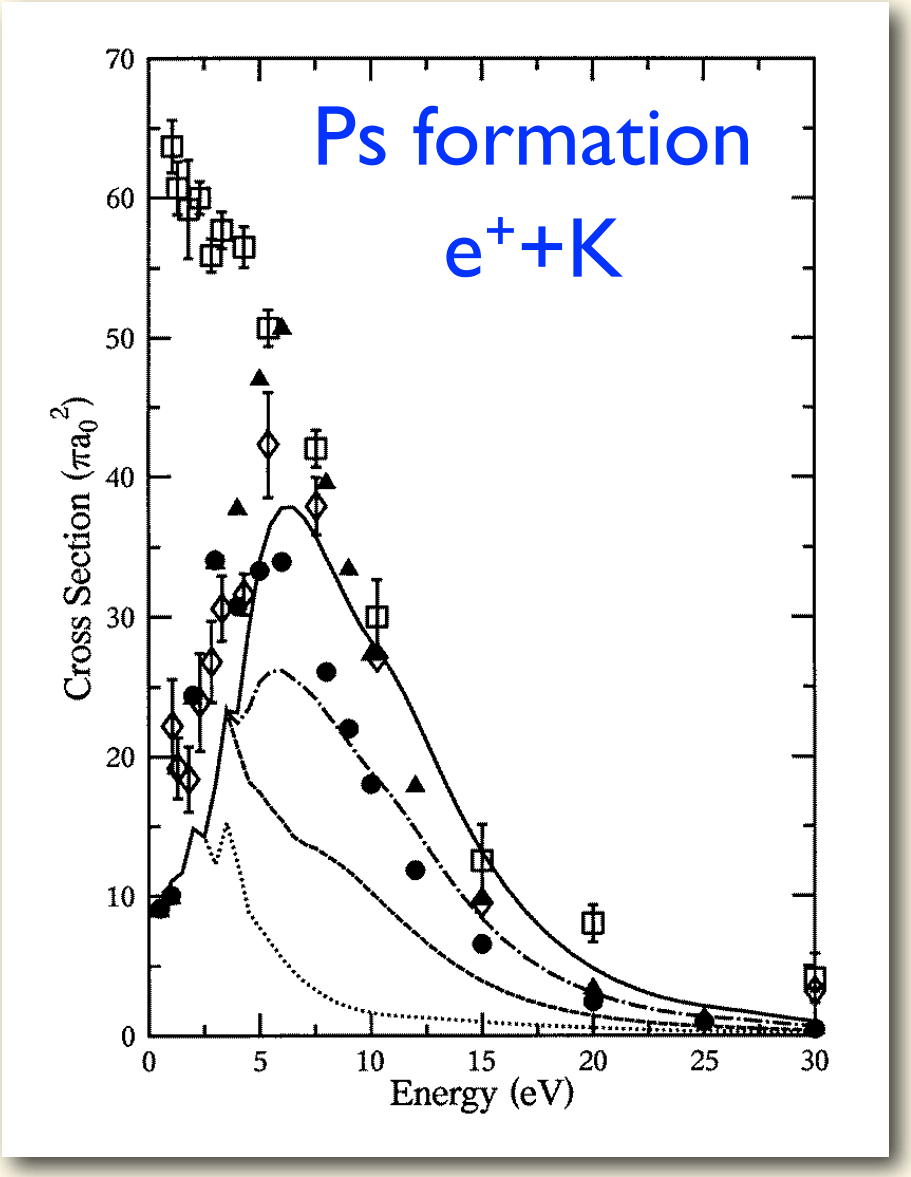
H. R. J. Walters *et al.*
Positron scattering from hydrogen and alkali atoms
J. Phys. B **28** 1079

1988-97

Positron scattering from alkali atoms

Ionization potential $I < 6.8$ eV



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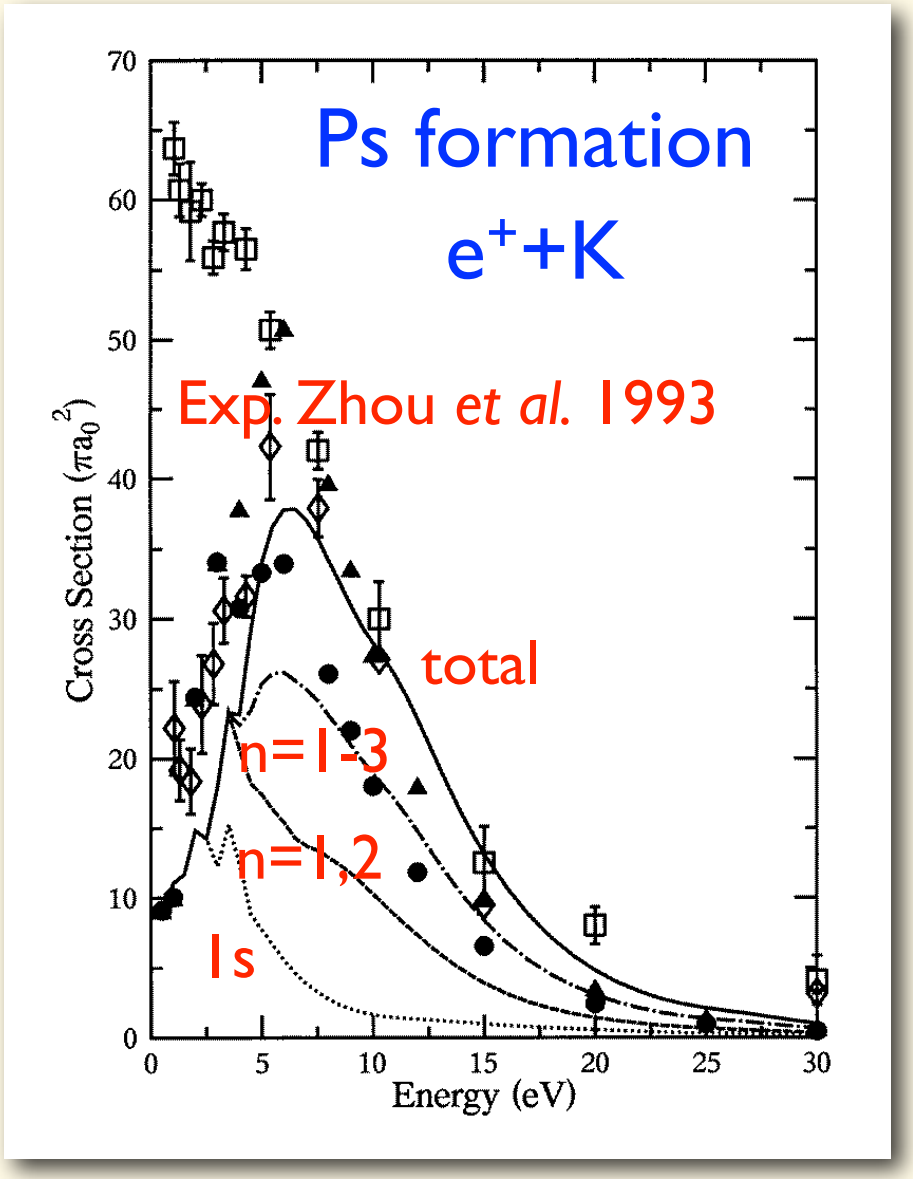

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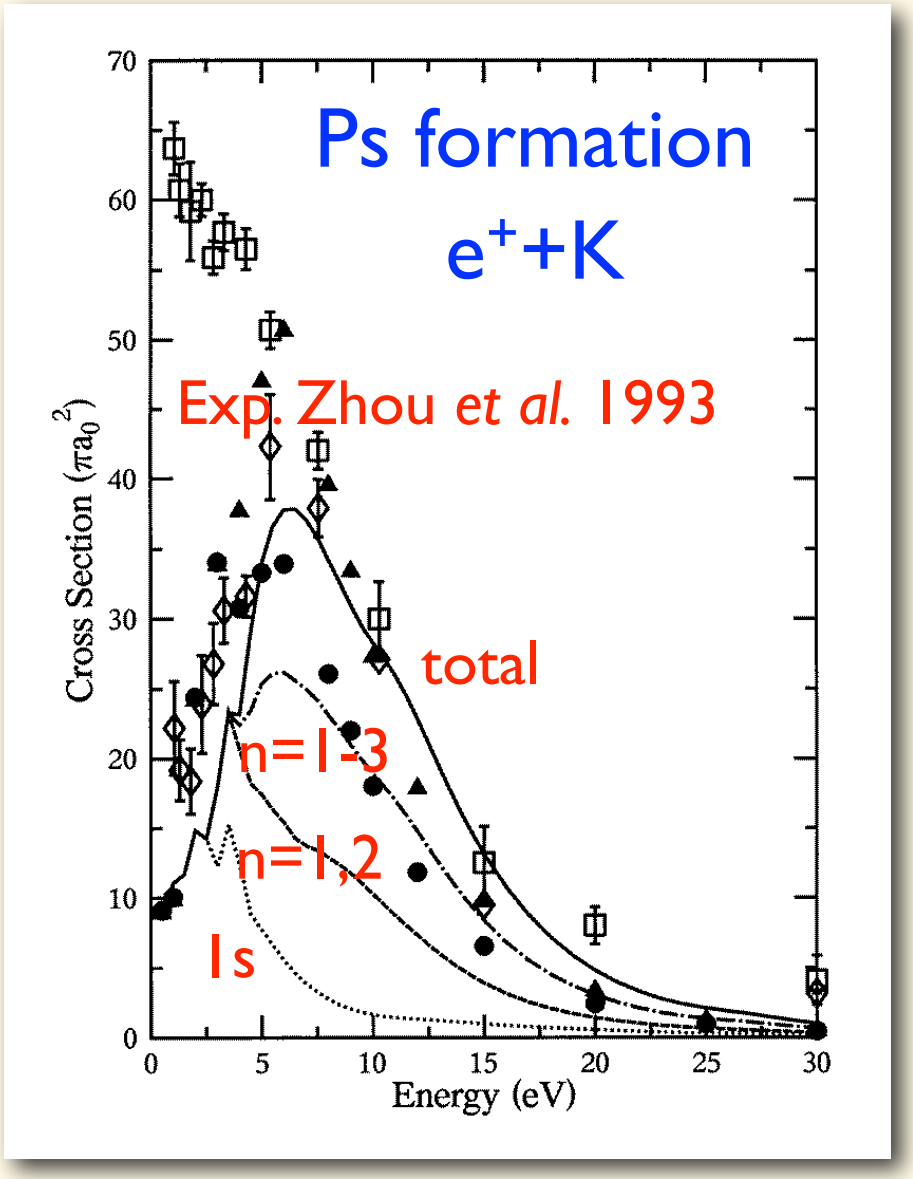

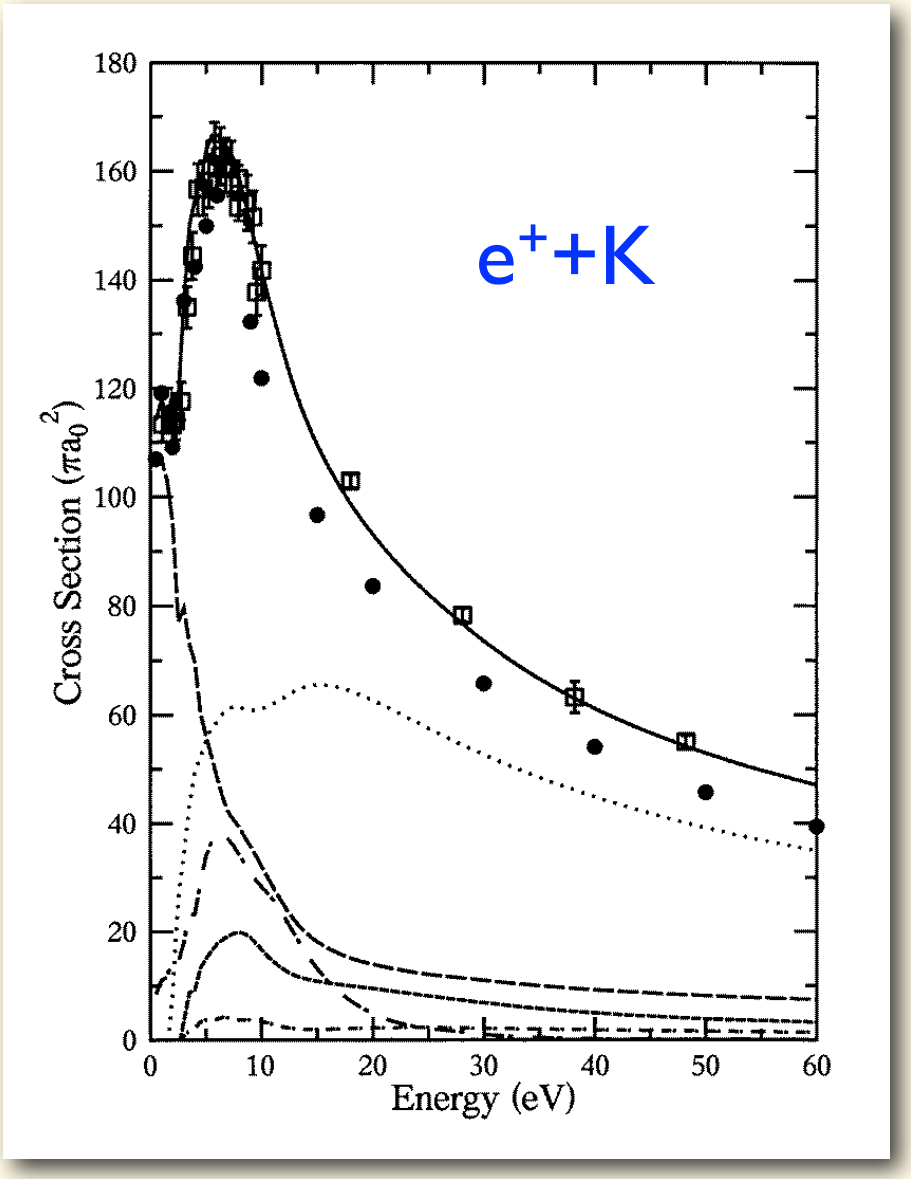

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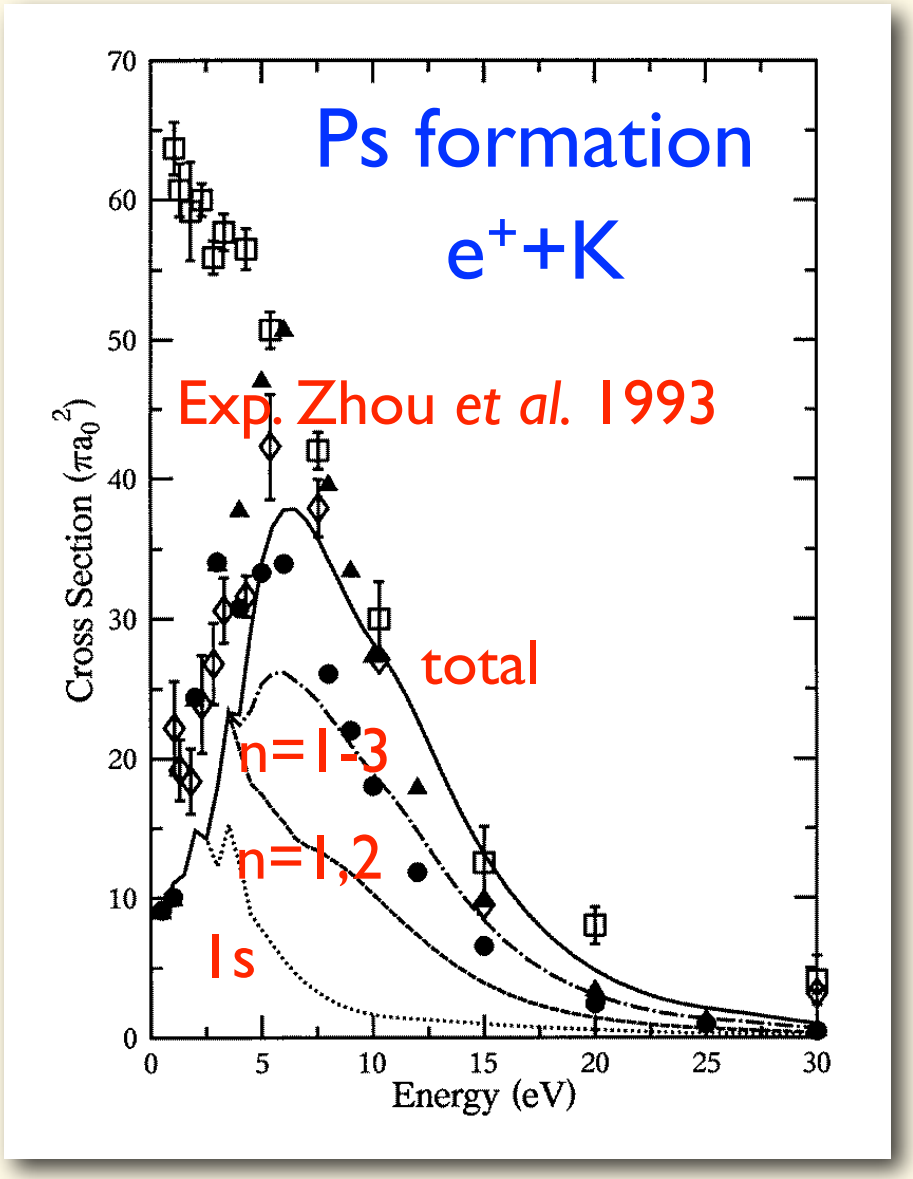

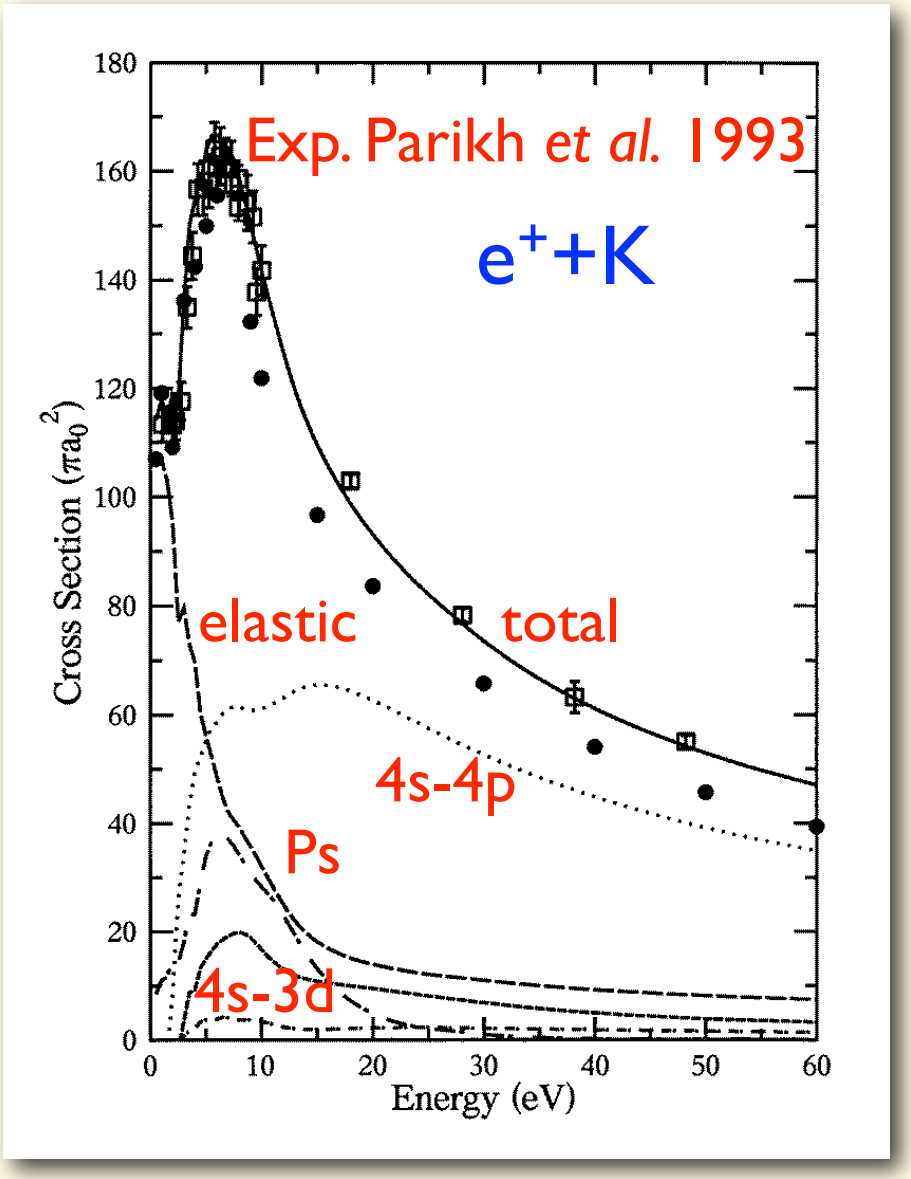

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Physics of positron-atom interaction

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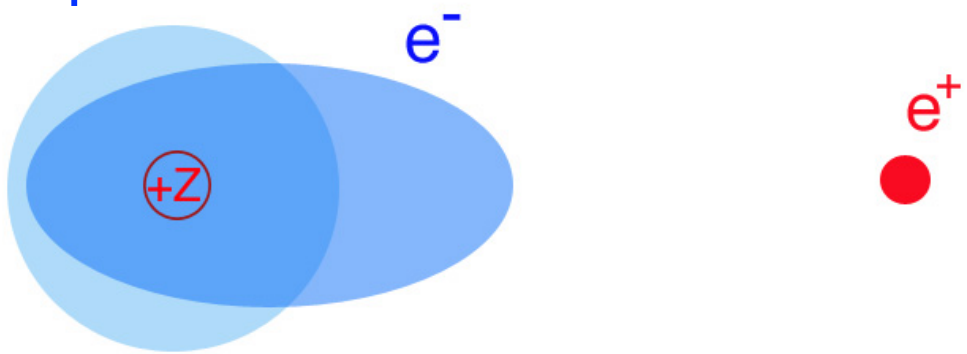
Large distances

target polarisation



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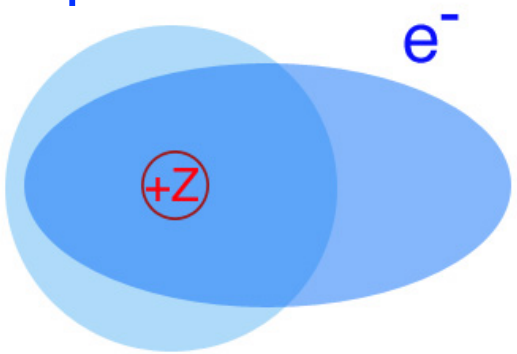

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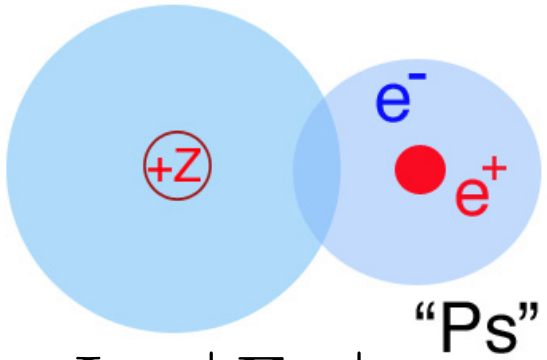
Atomic-size distances

virtual Ps formation



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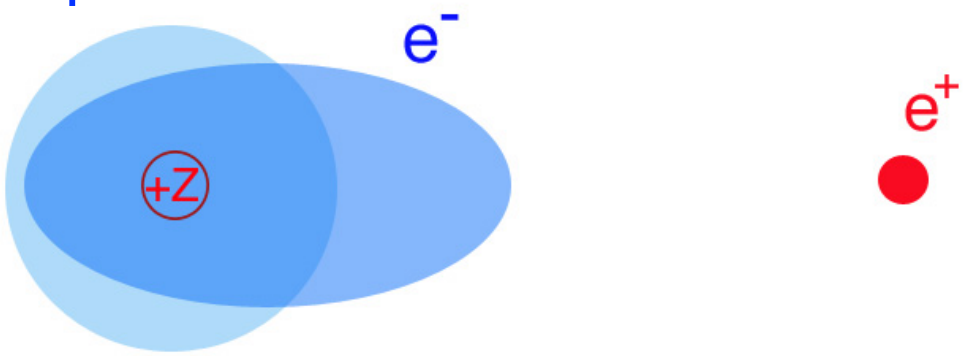

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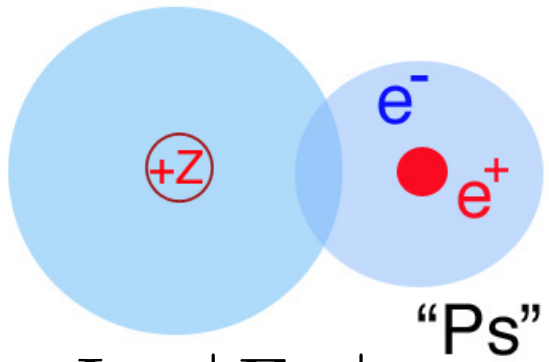

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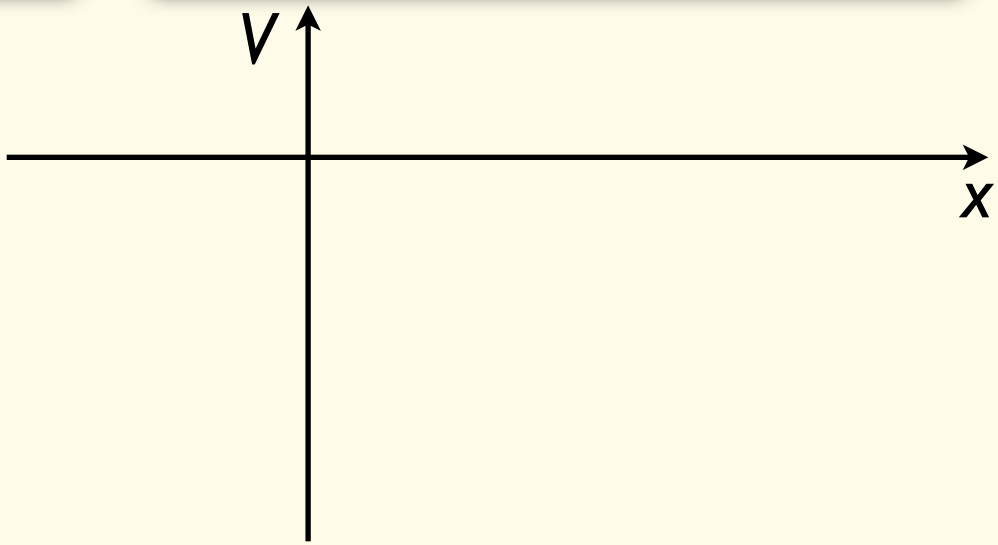

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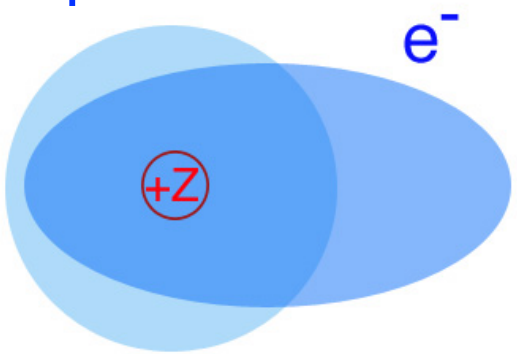

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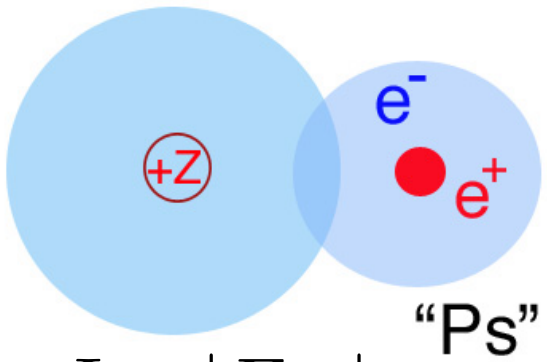

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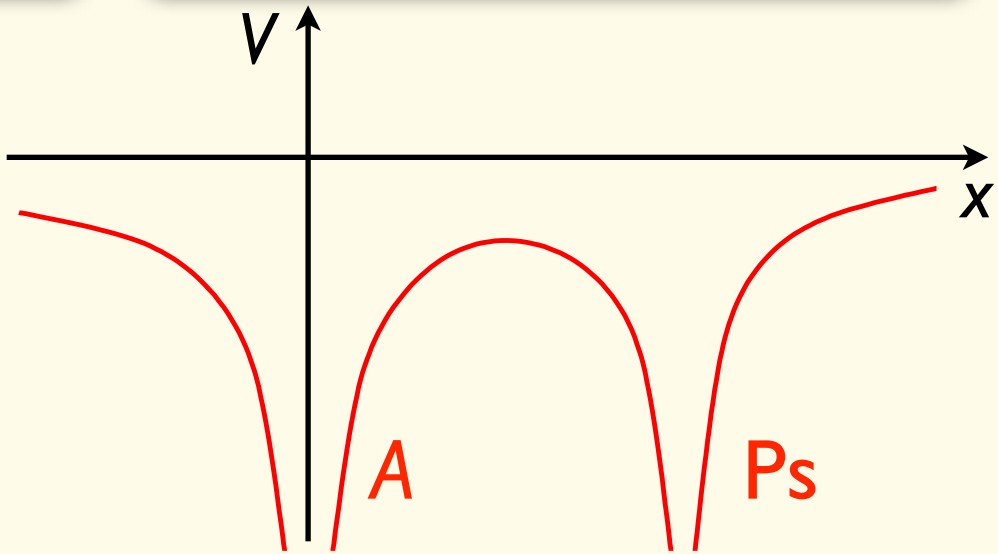

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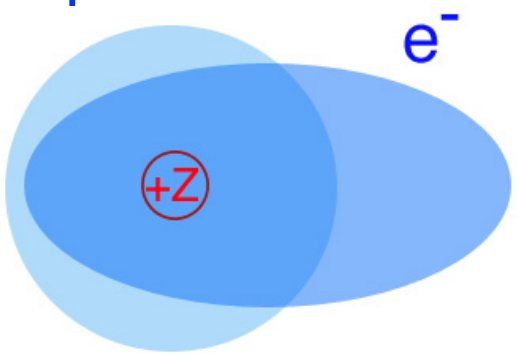

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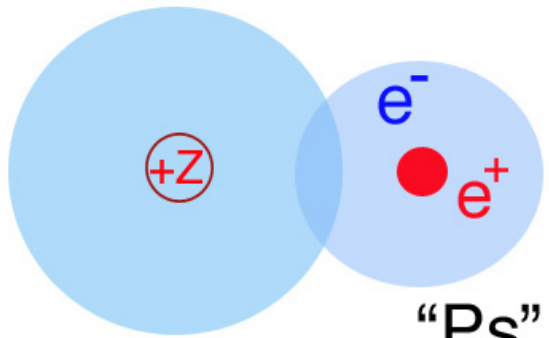

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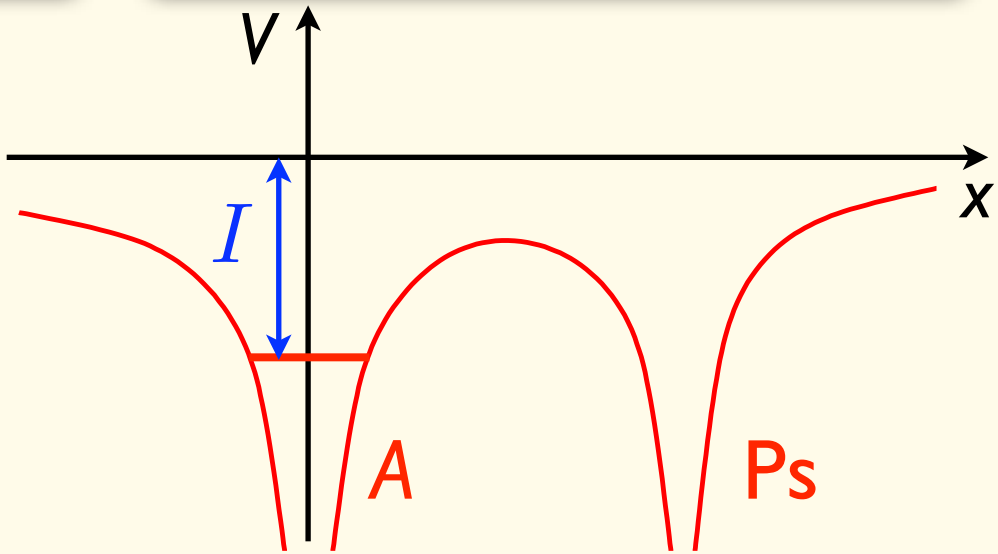

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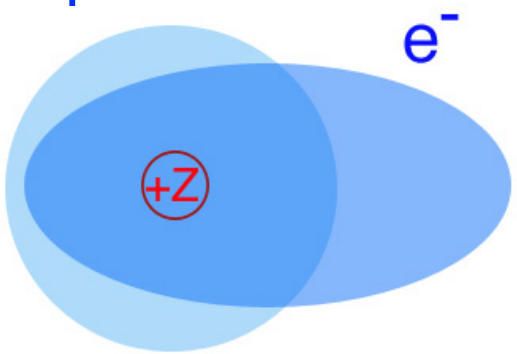

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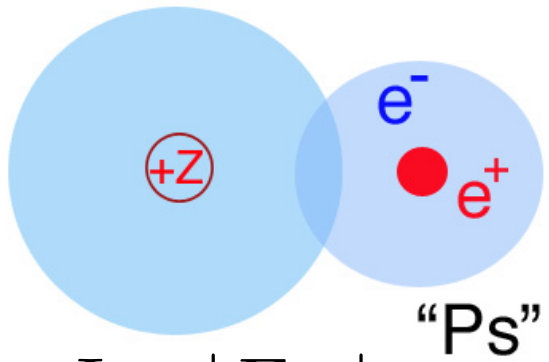

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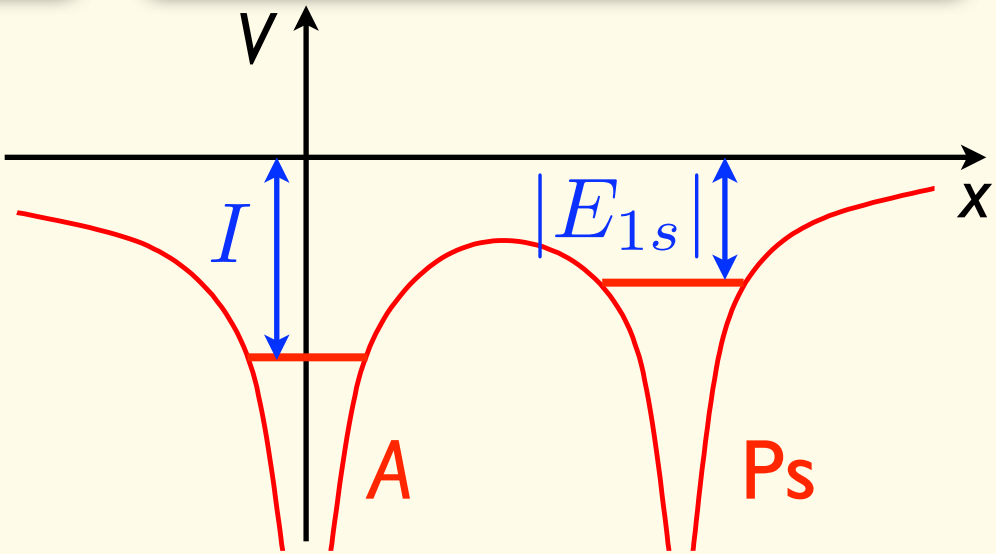


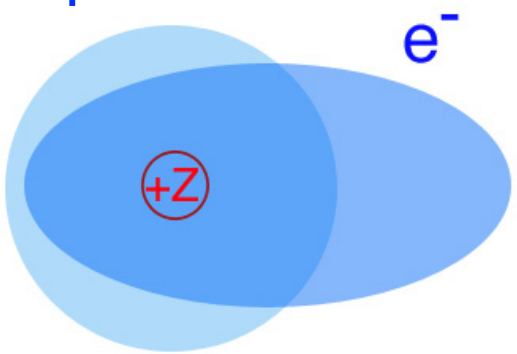
Physics of positron-atom interaction

Small distances - repulsive electrostatic potential

$$\sim Z/r \;\; \text{at} \;\; r \ll a_B$$

Large distances

target polarisation



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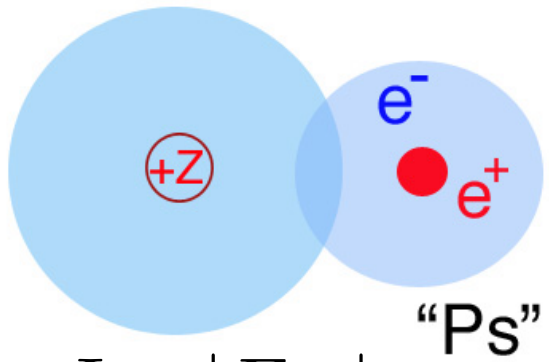

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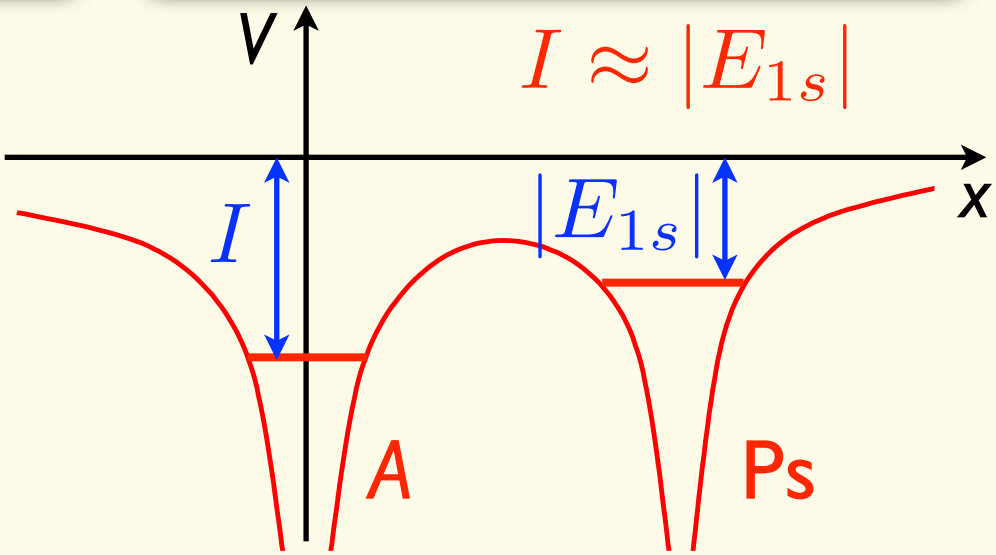

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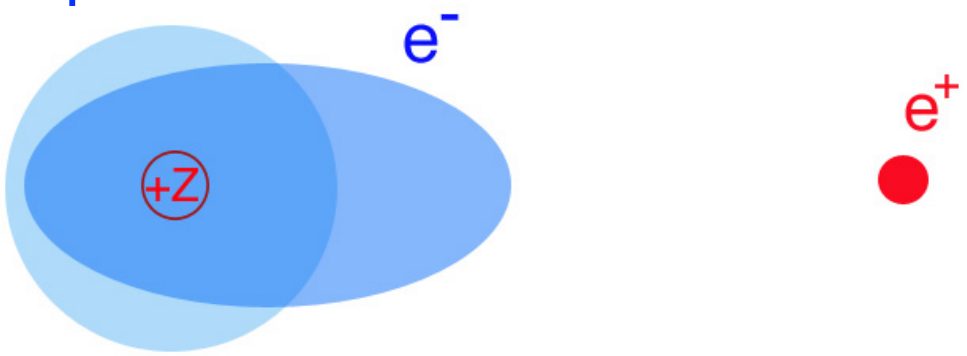

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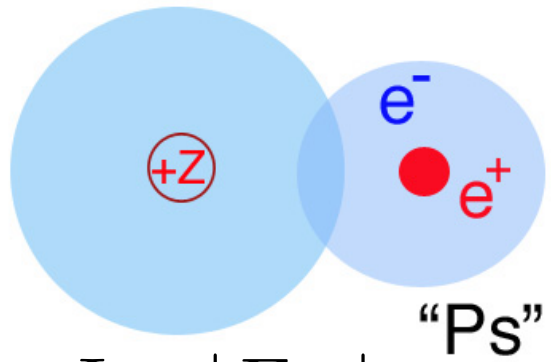

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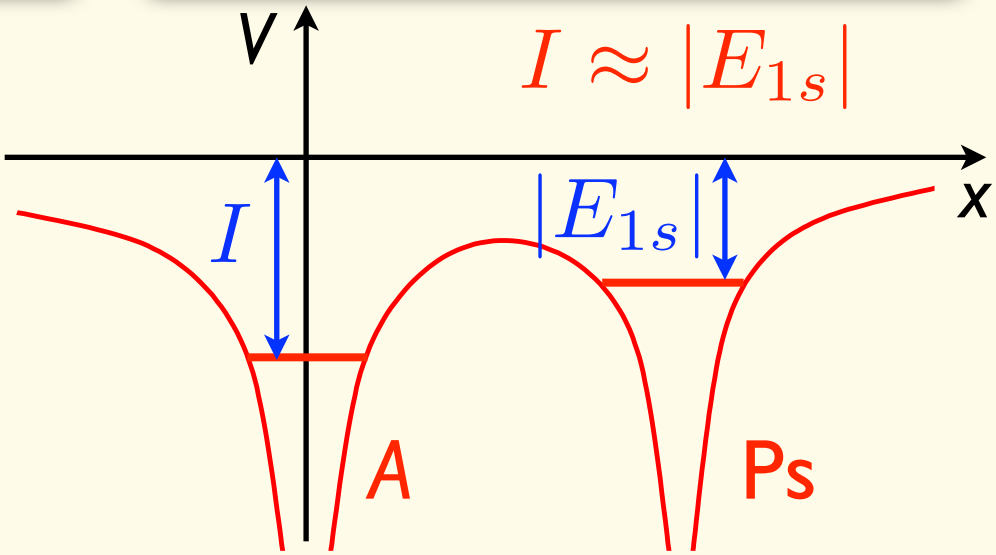
Attraction!



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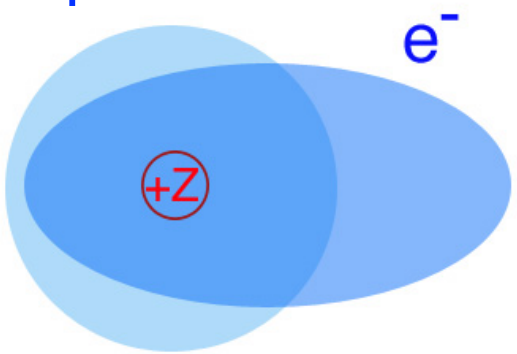

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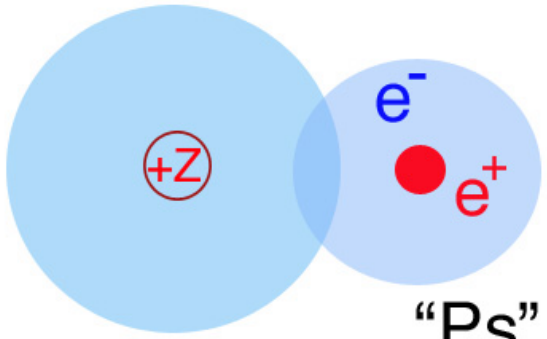

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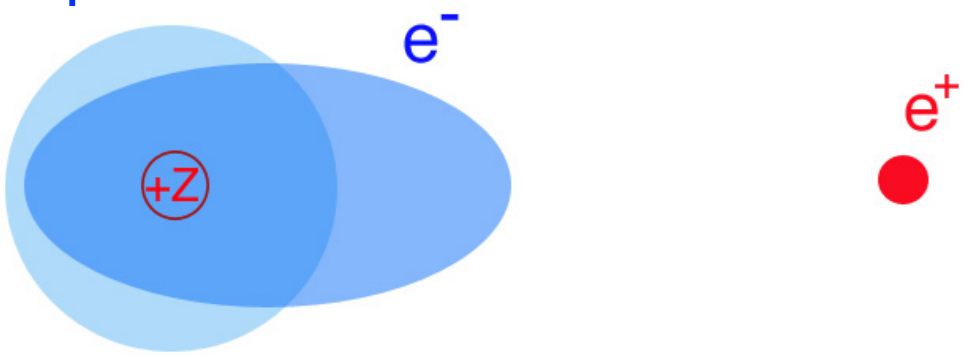

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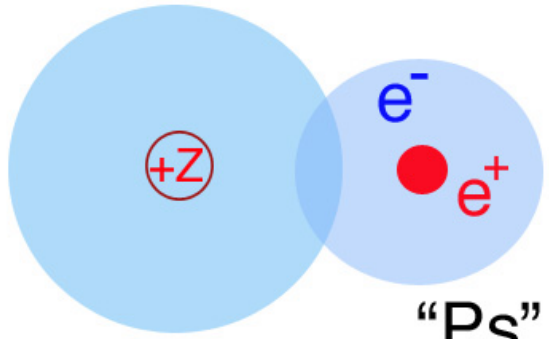

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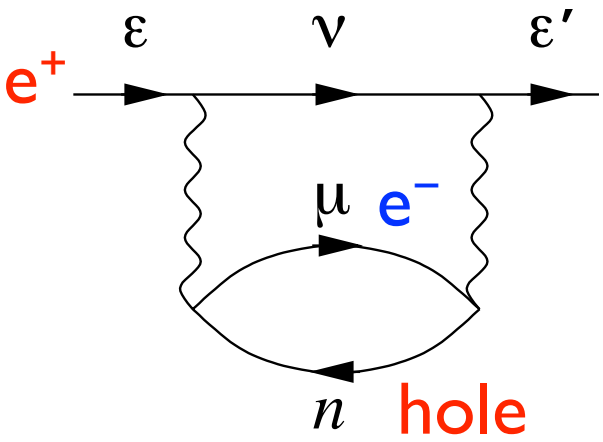

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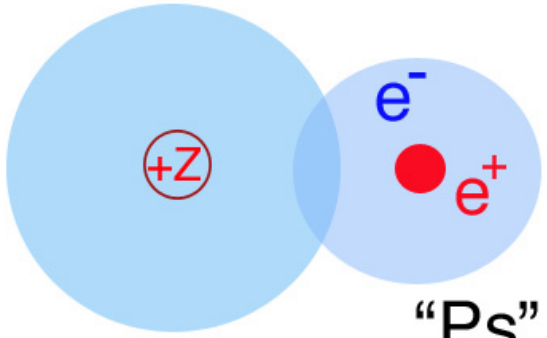

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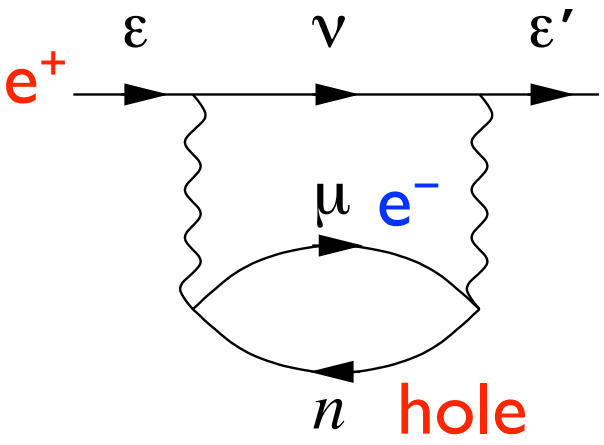

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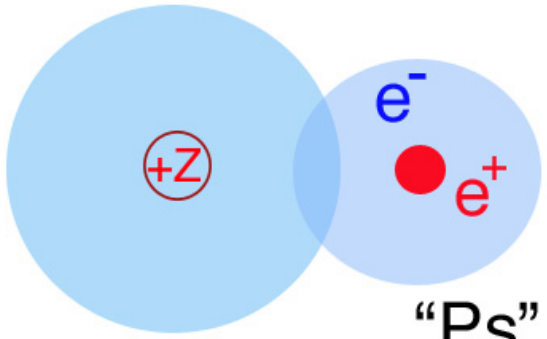

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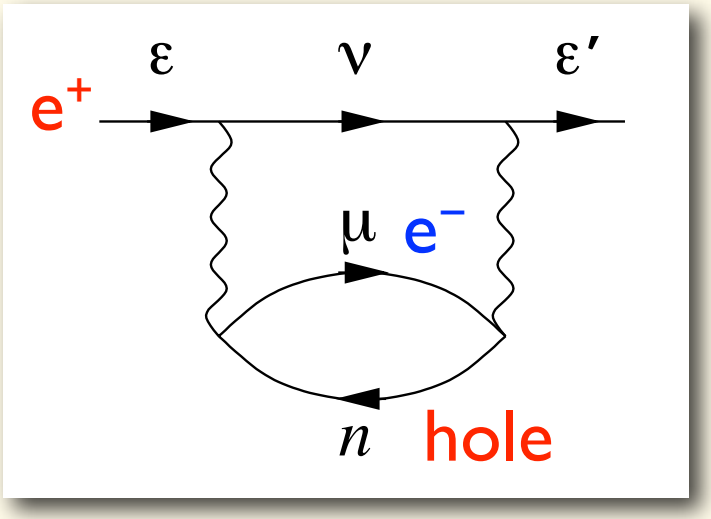

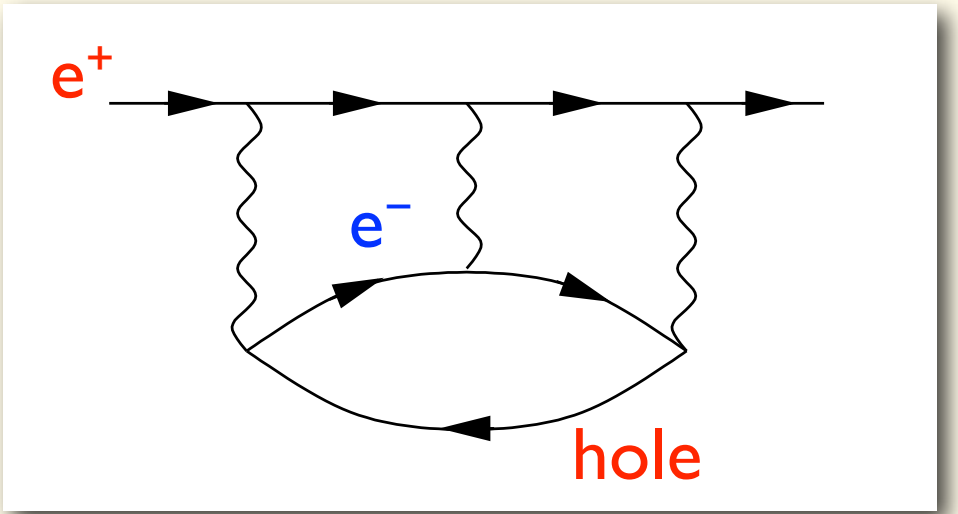

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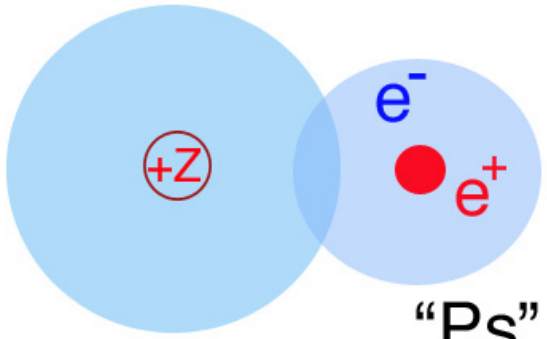

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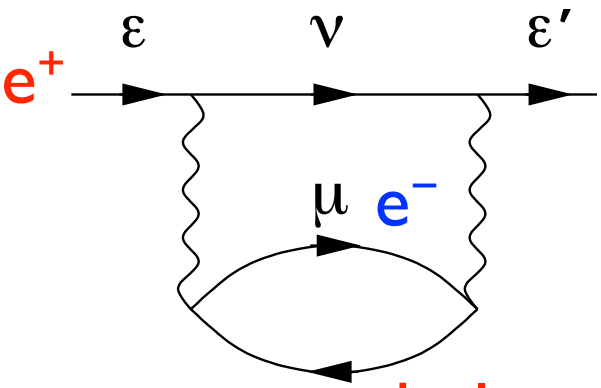

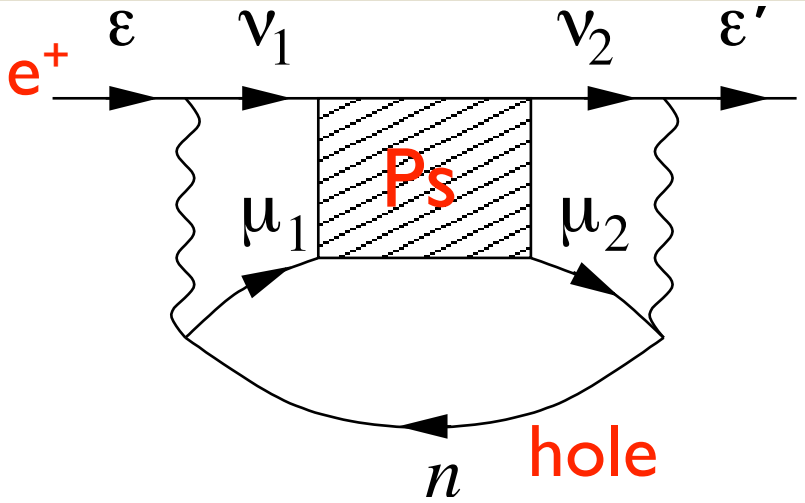

Dyson equation

$$H_0\varphi_\varepsilon(\mathbf{r}) + \int \Sigma_\varepsilon(\mathbf{r},\mathbf{r}')\varphi_\varepsilon(\mathbf{r}')d\mathbf{r}' = \varepsilon\varphi_\varepsilon(\mathbf{r})$$

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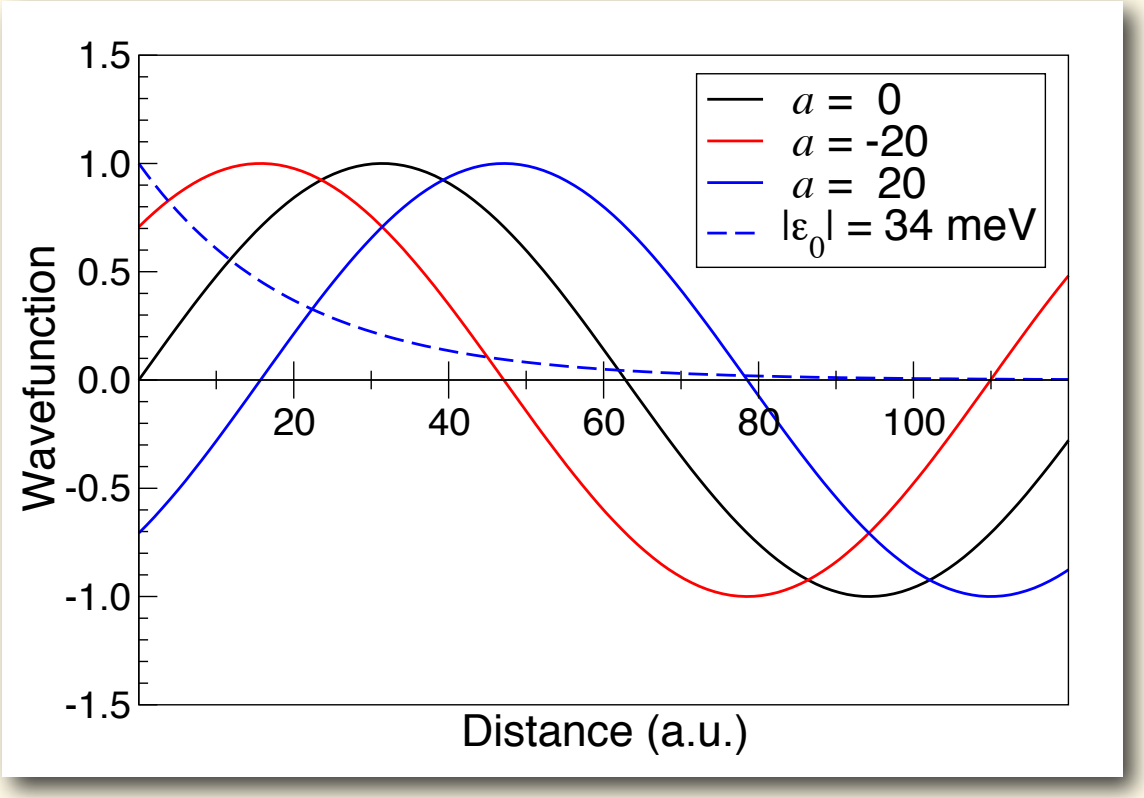

Low-energy $kR_a \ll 1$

e.g. thermal at 300 K

$k = 0.05$ a.u.

s-wave ($l = 0$) dominates

$\varphi \propto \sin(kr + \delta_0)$

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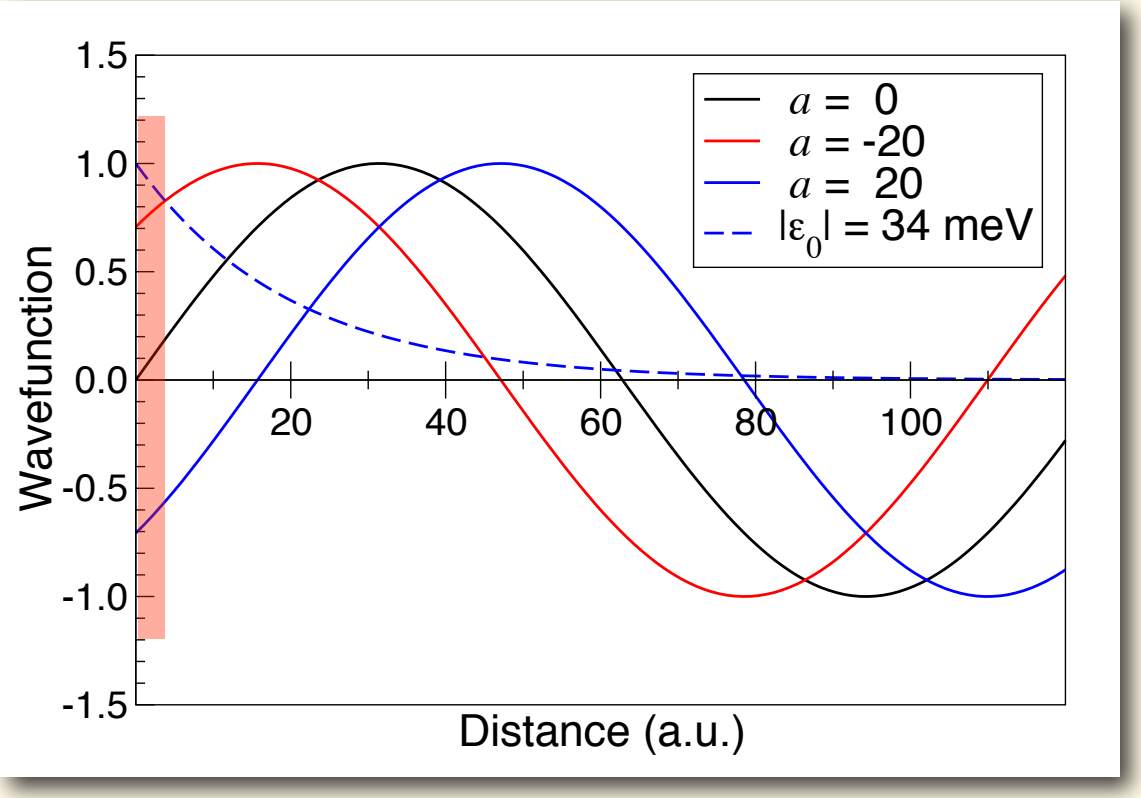

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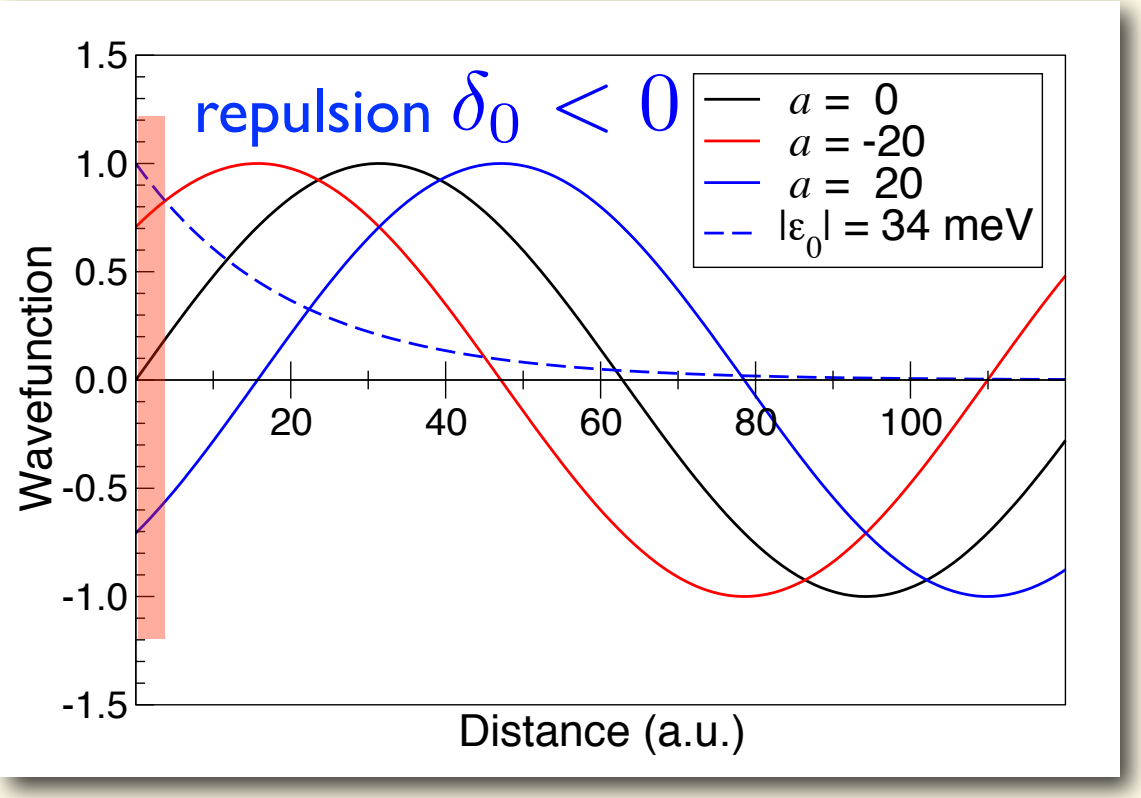

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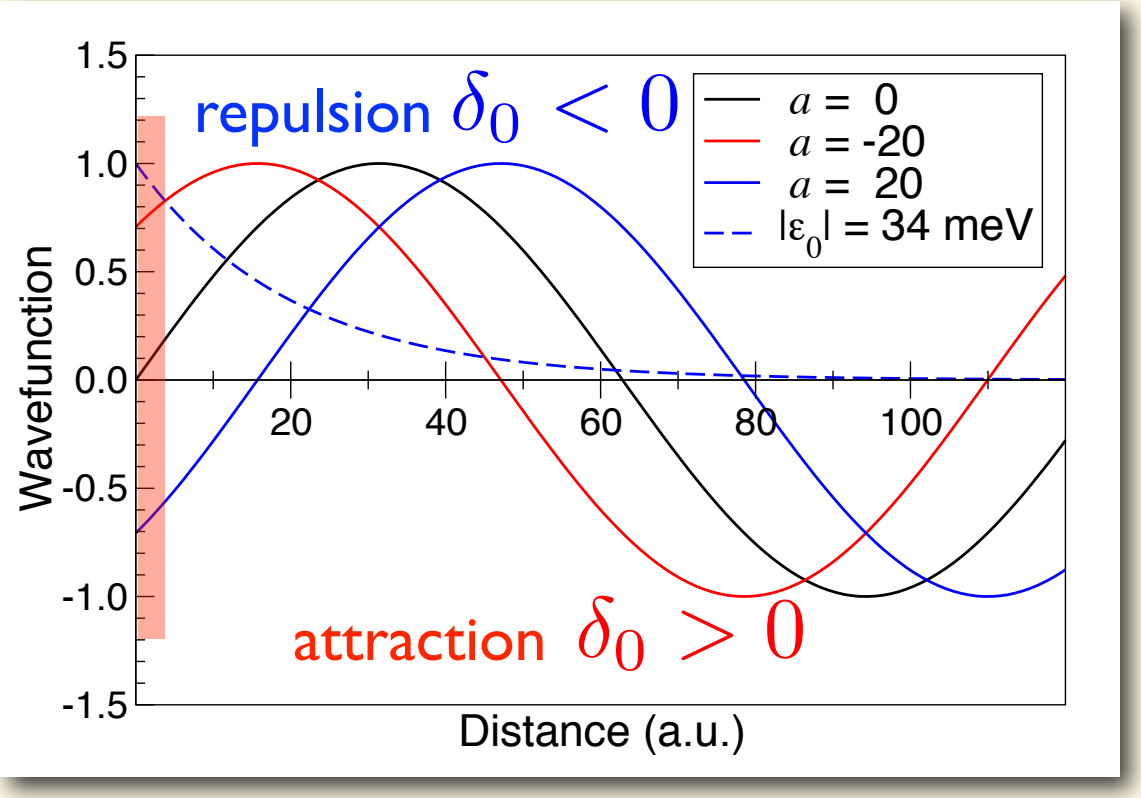

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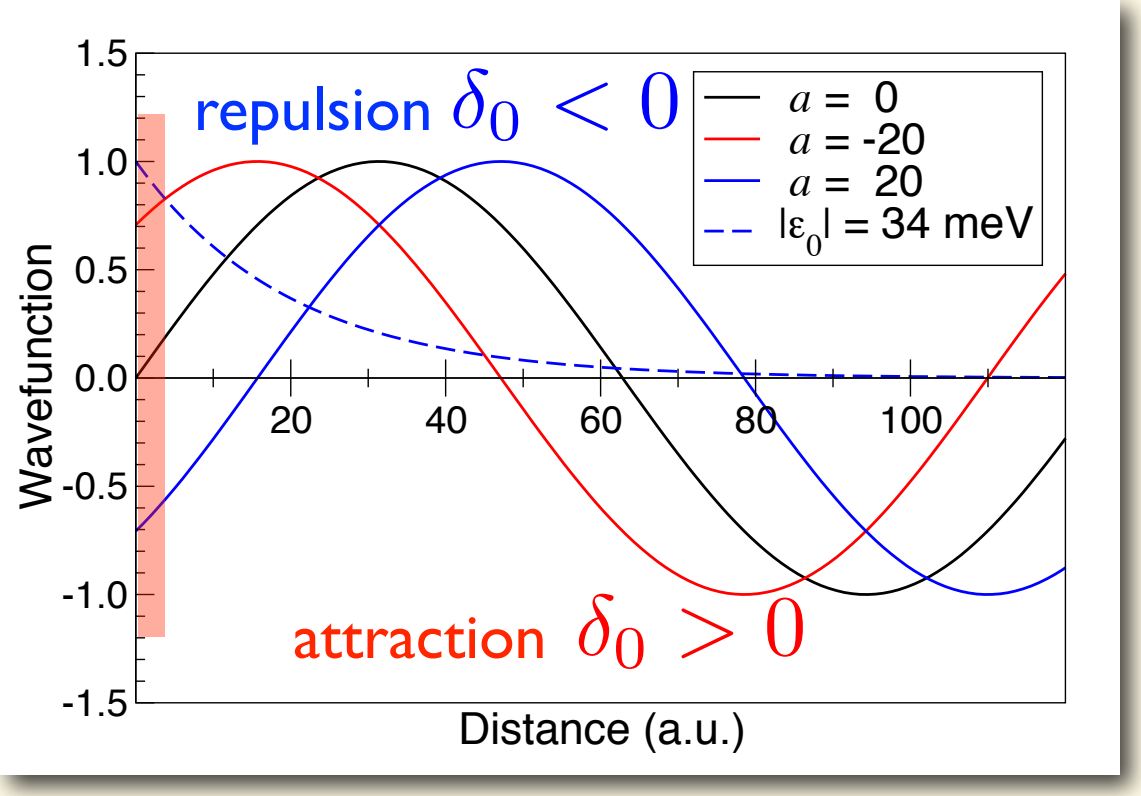

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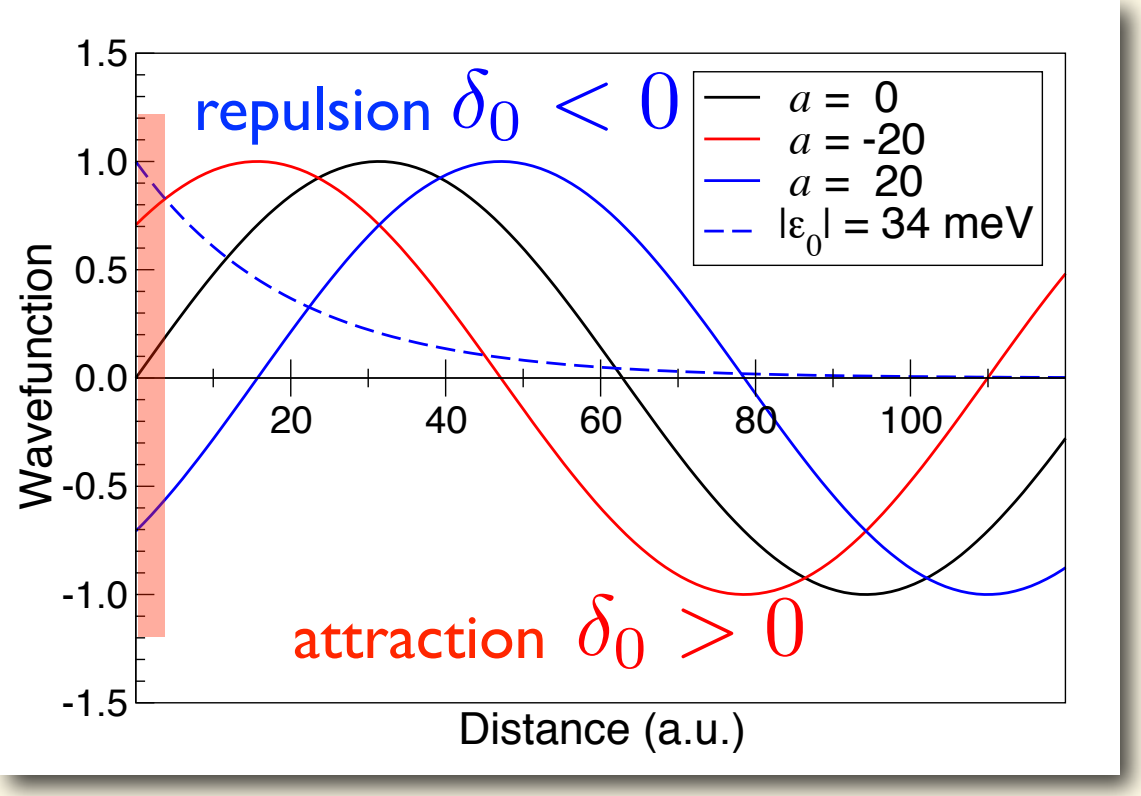

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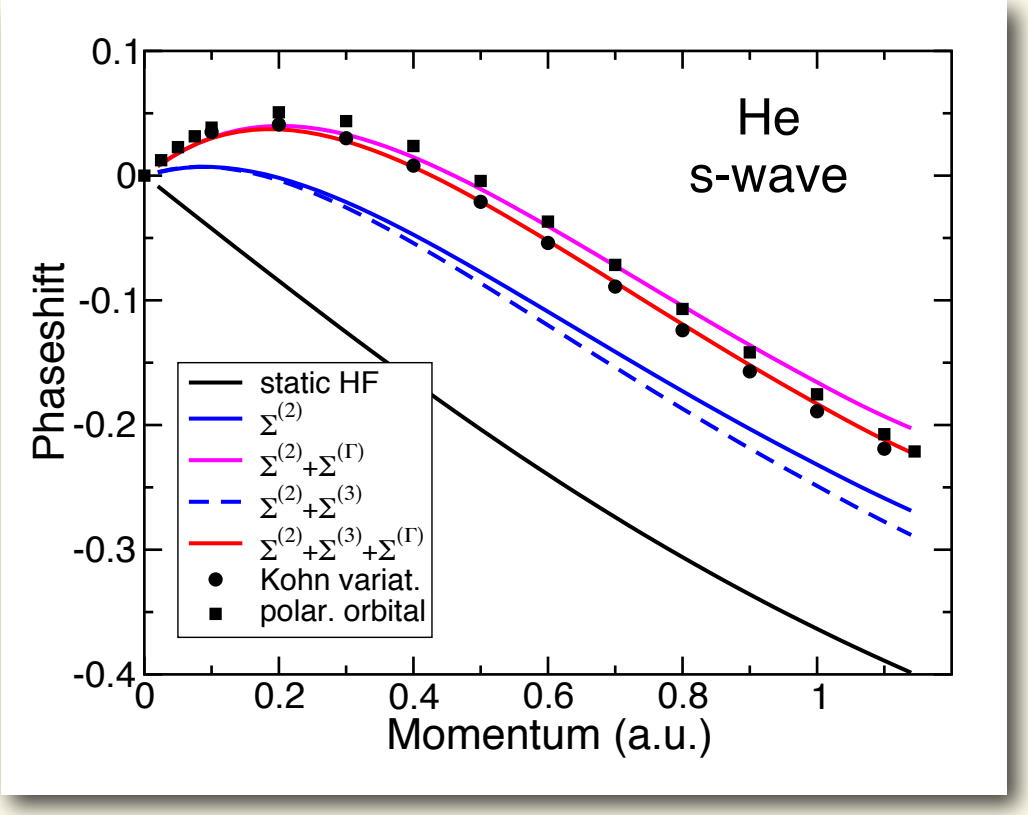
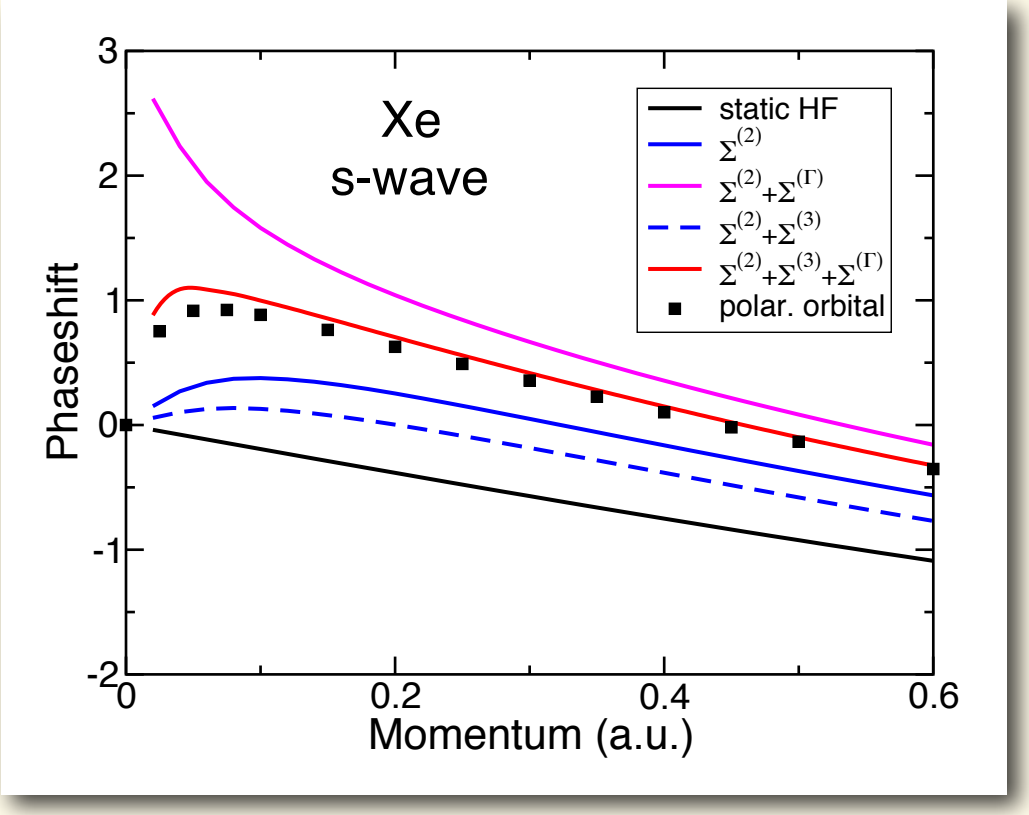
scattering length

Positron scattering from noble gas atoms





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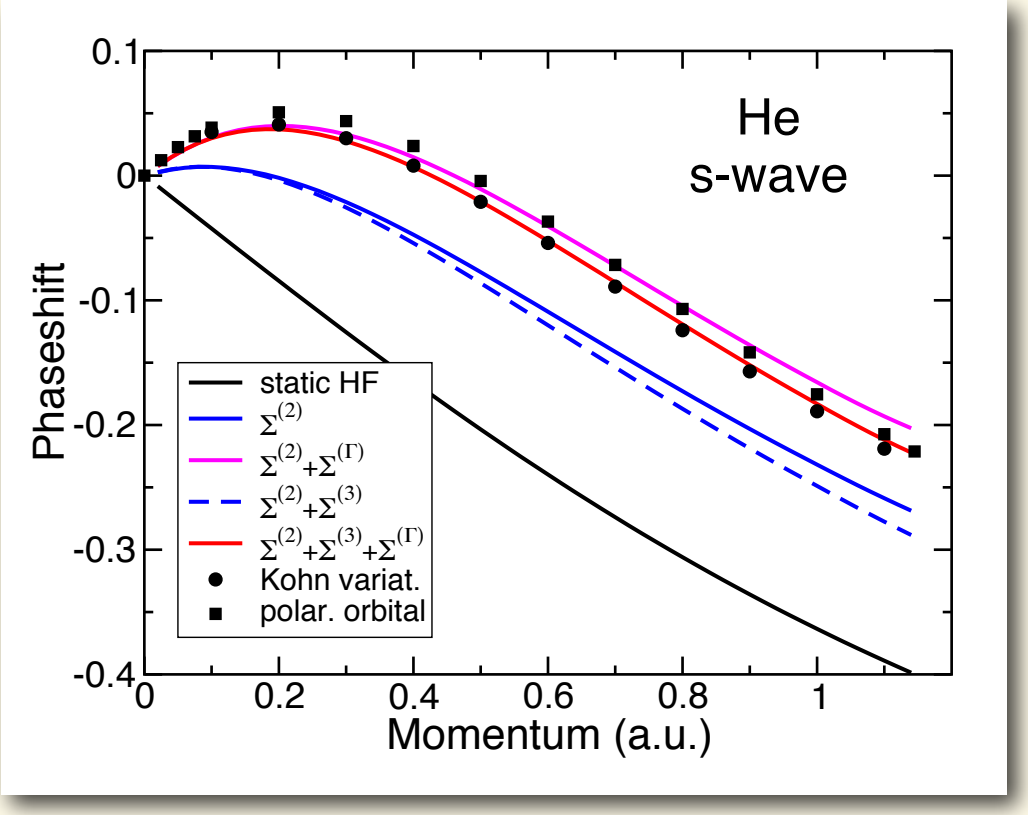

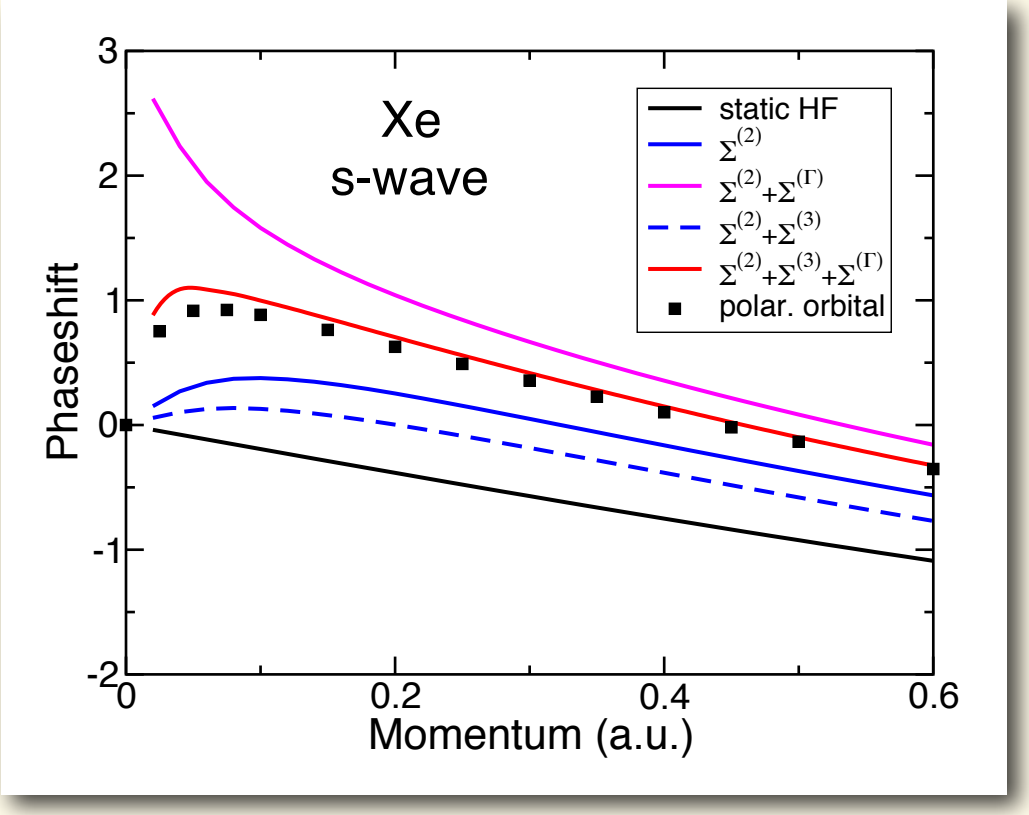

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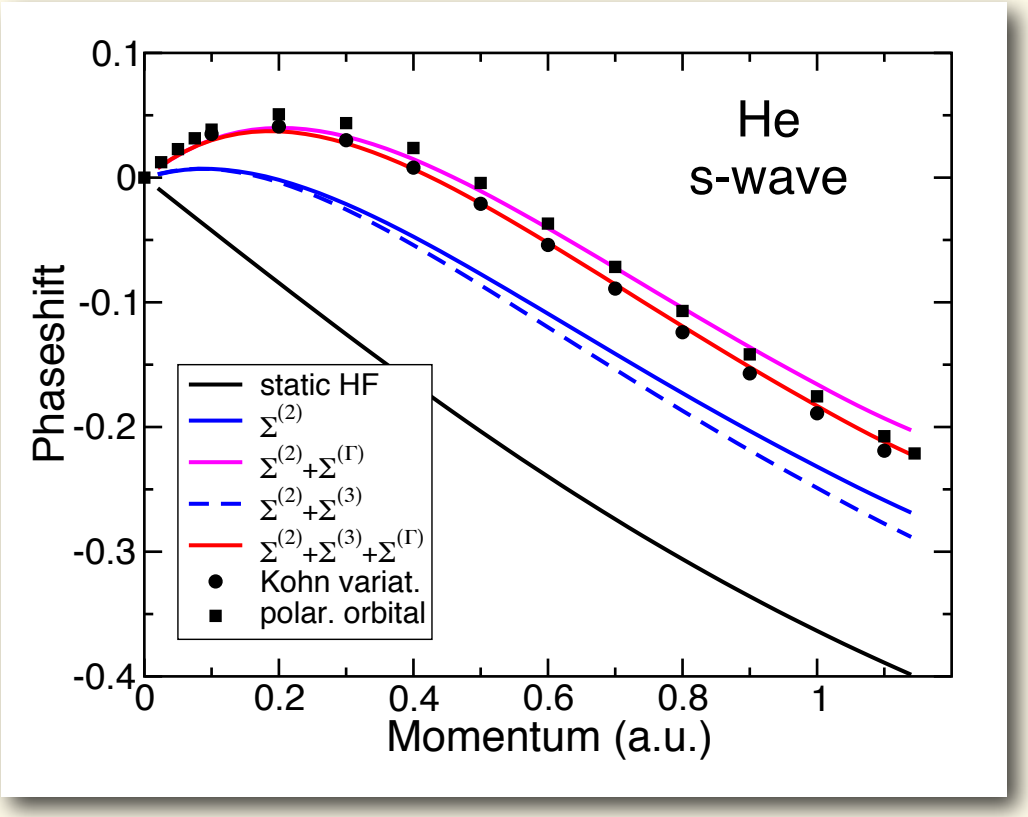

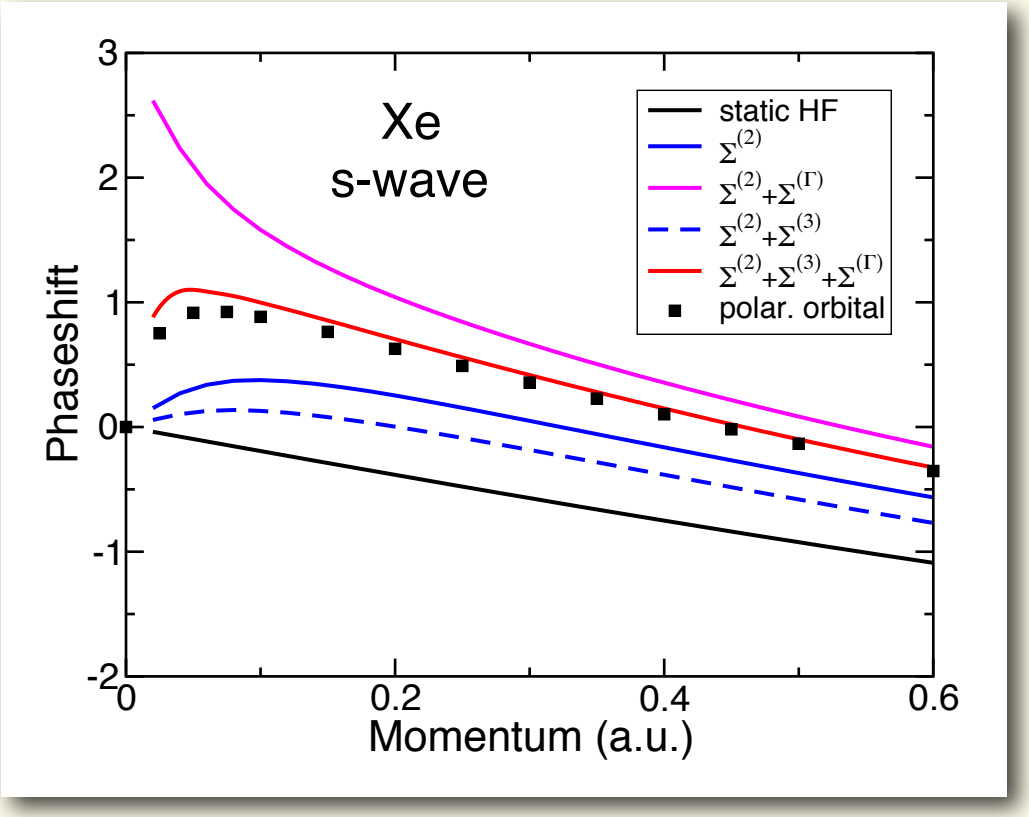

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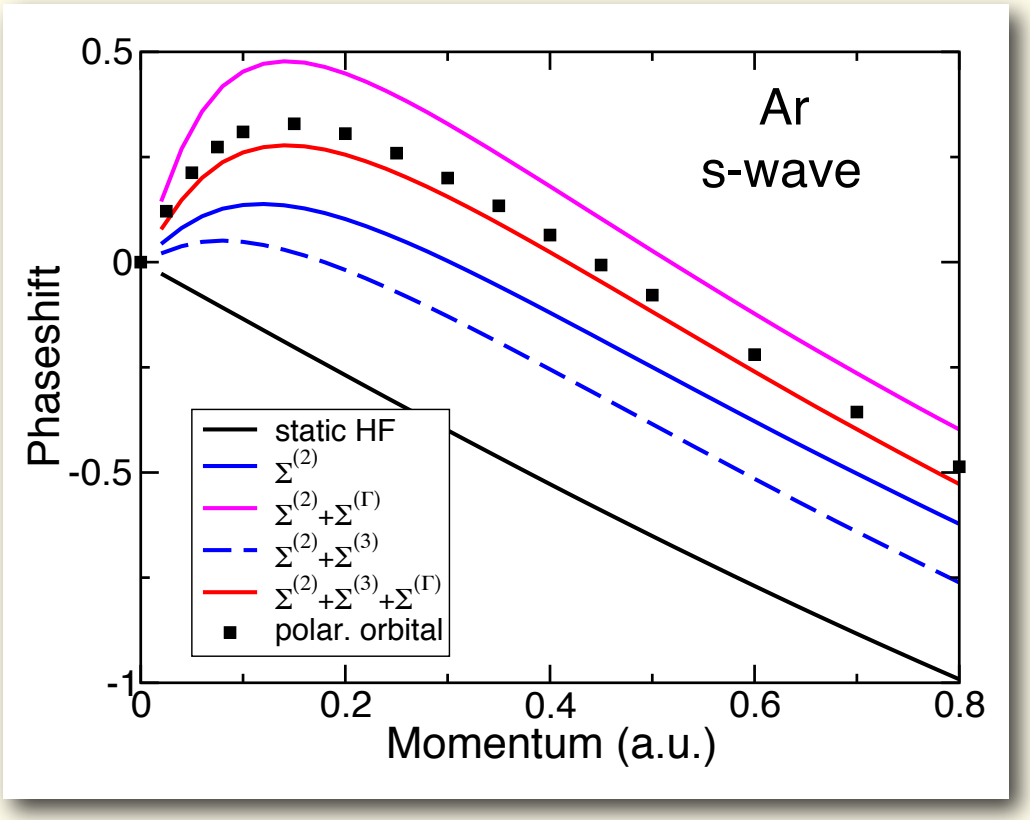
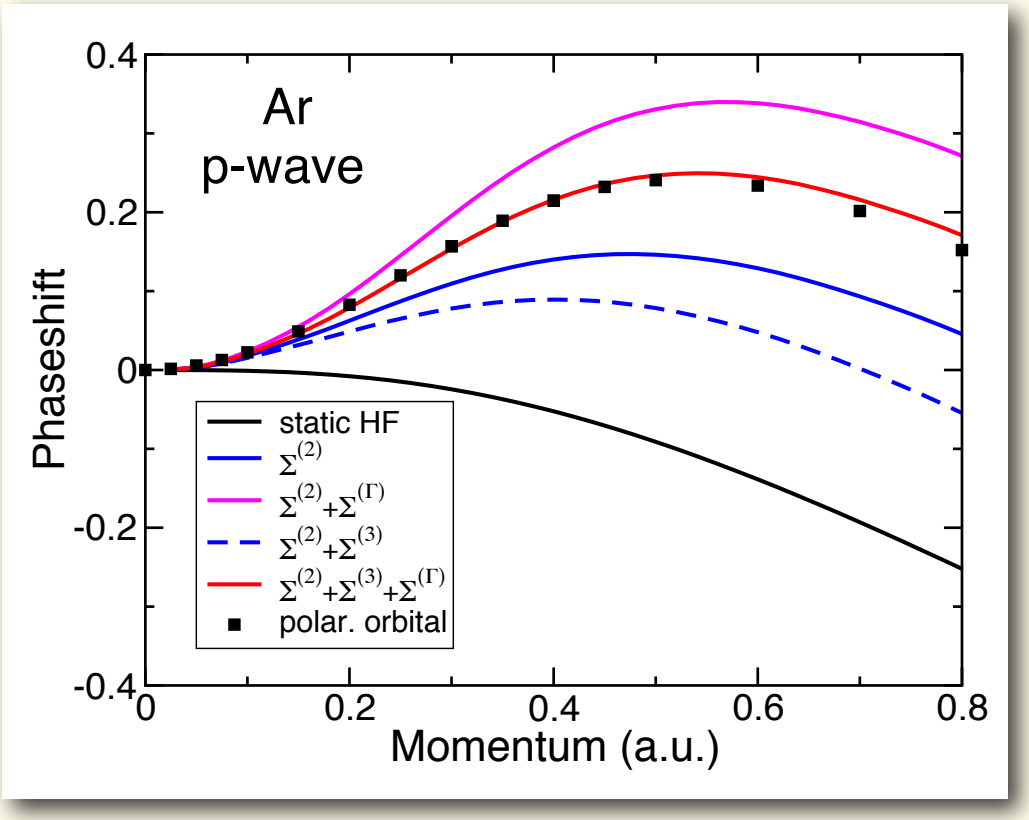
Correlations change the scattering length from positive (static repulsion) to negative

Positron scattering from noble gas atoms





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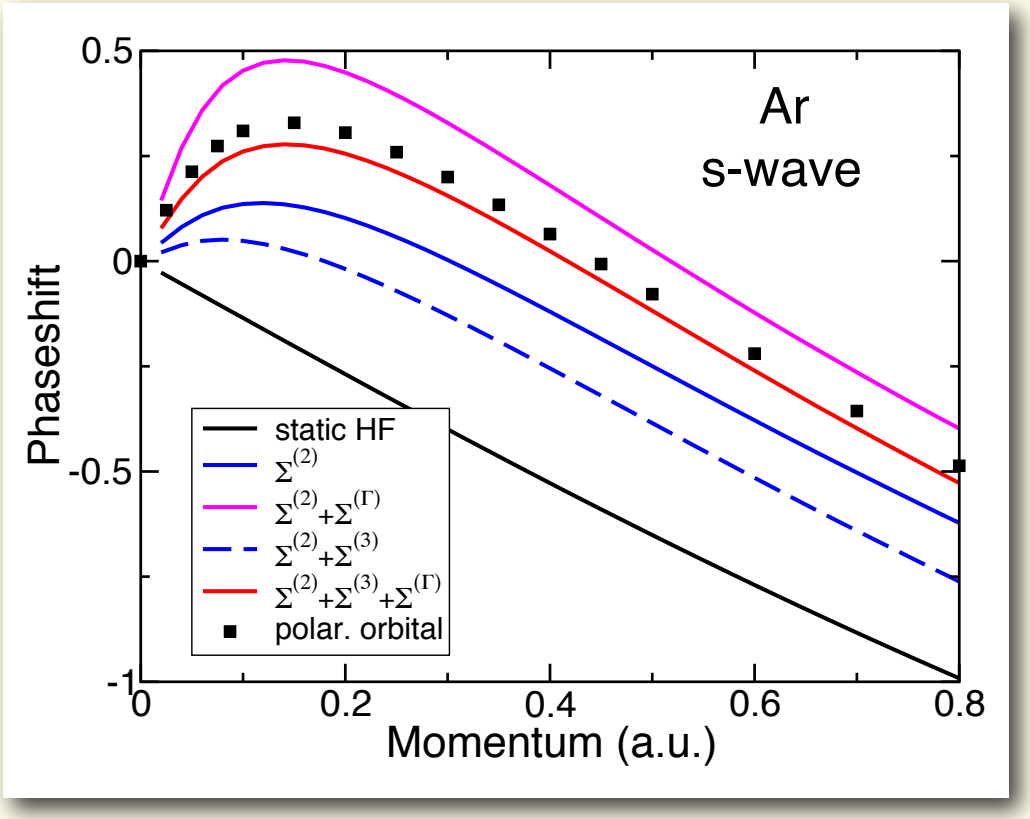

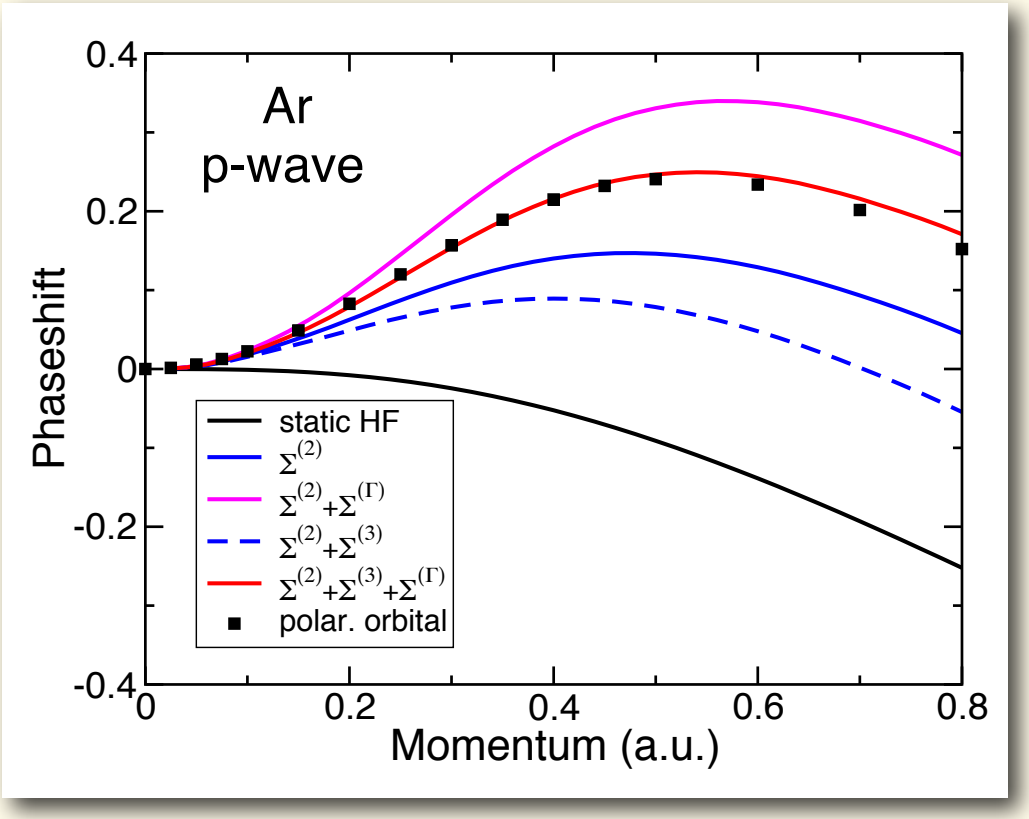

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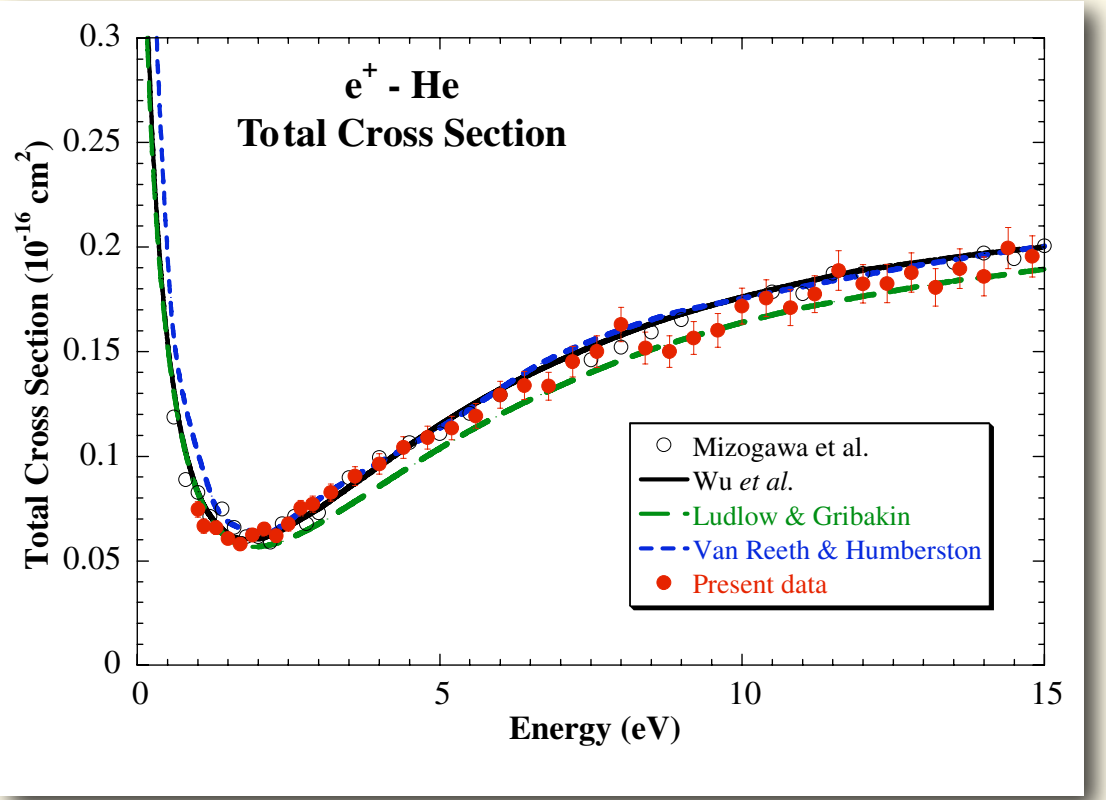
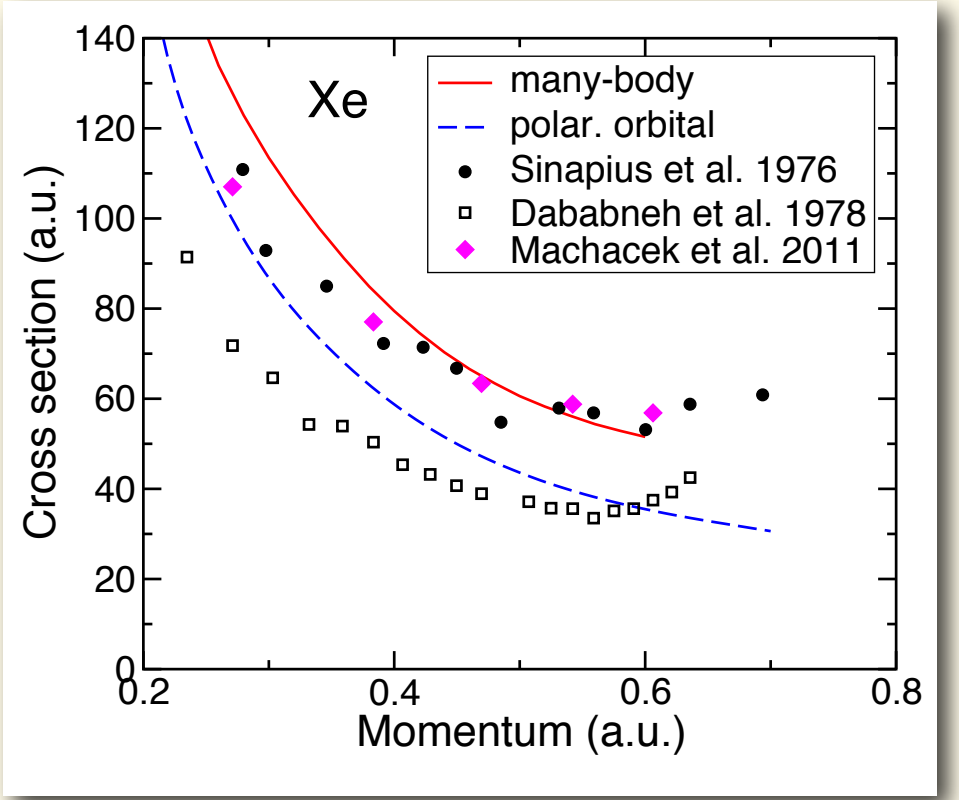
Higher partial waves also show attraction

Comparison between theory and experiment





Sullivan *et al.* J. Phys. B **41** 081001 (2008)

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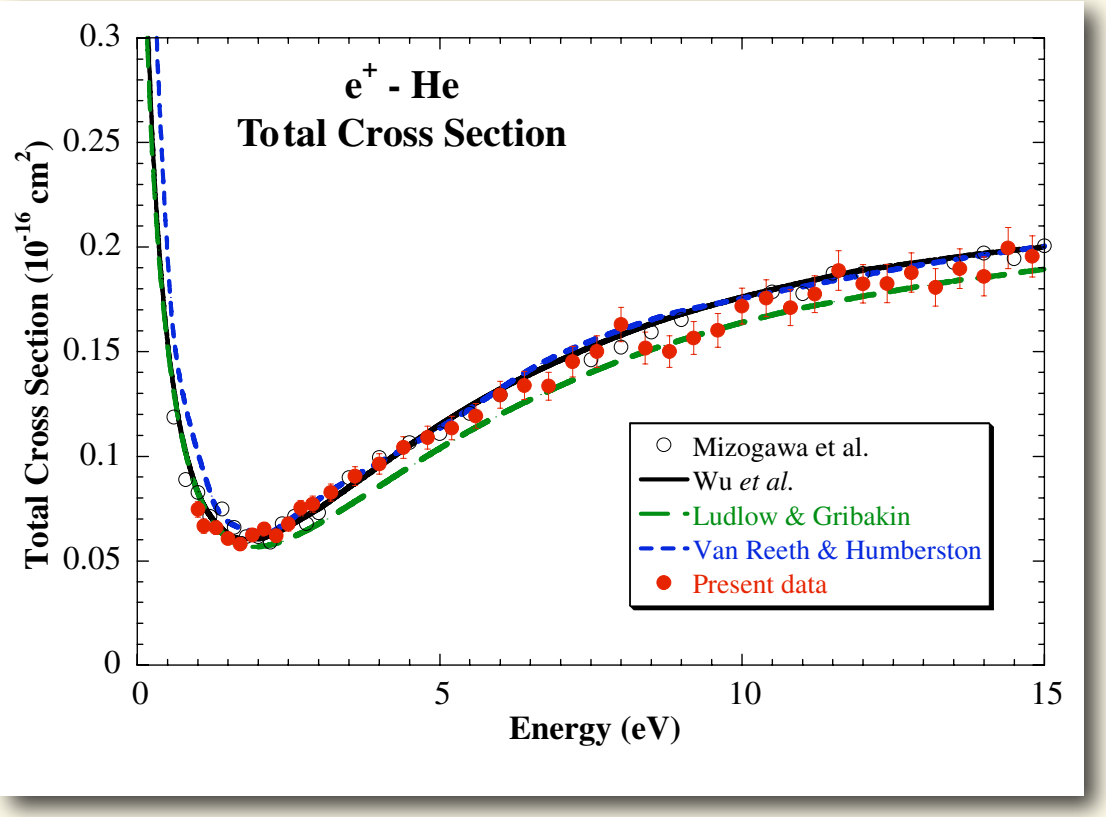

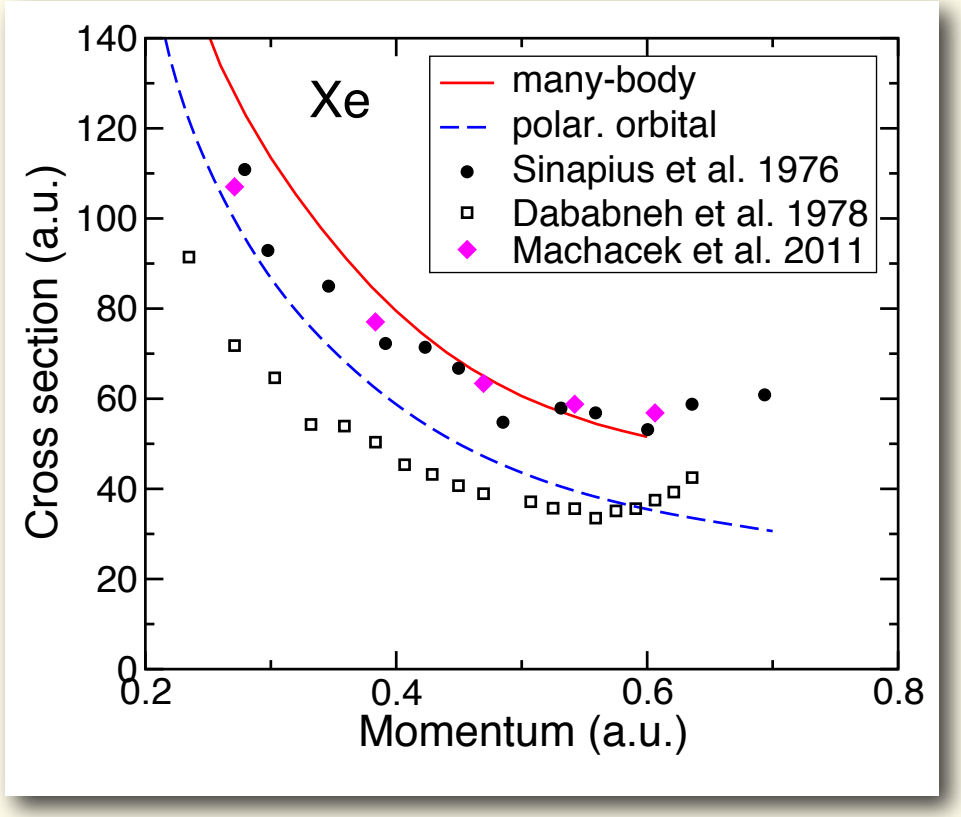

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Cross sections at low energies increase greatly from He to Xe. Positron-atom attraction creates virtual s-levels in heavier atoms, at $\varepsilon = 1/2a^2$

	He	Ne	Ar	Kr	Xe
scattering length (a.u.)	−0.42	−0.43	−4.4	−10.1	−81
virtual level energy (eV)	–	–	0.7	0.13	0.002

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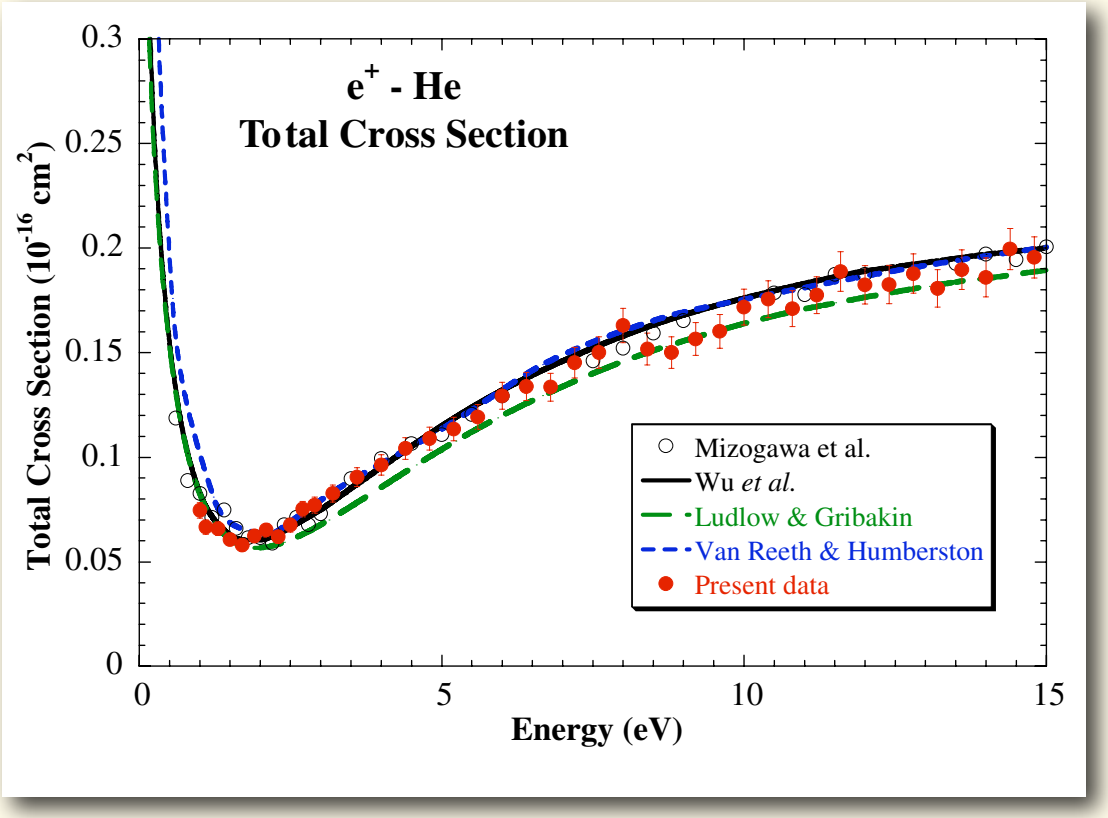

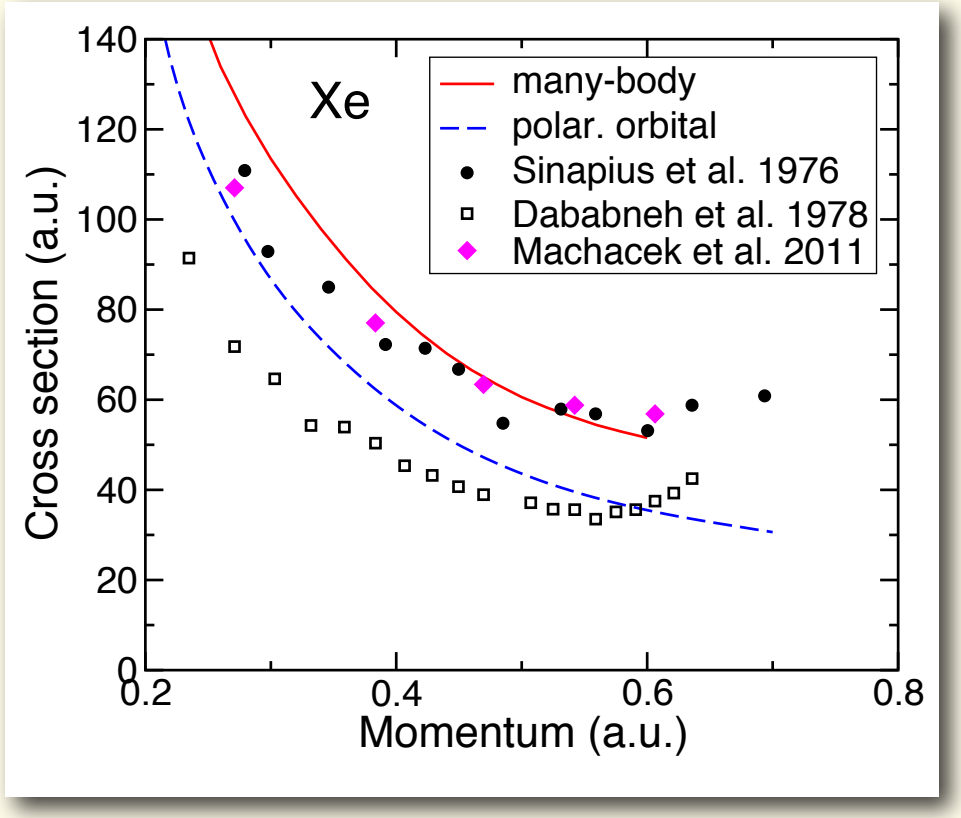

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Positron-atom binding

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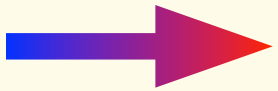
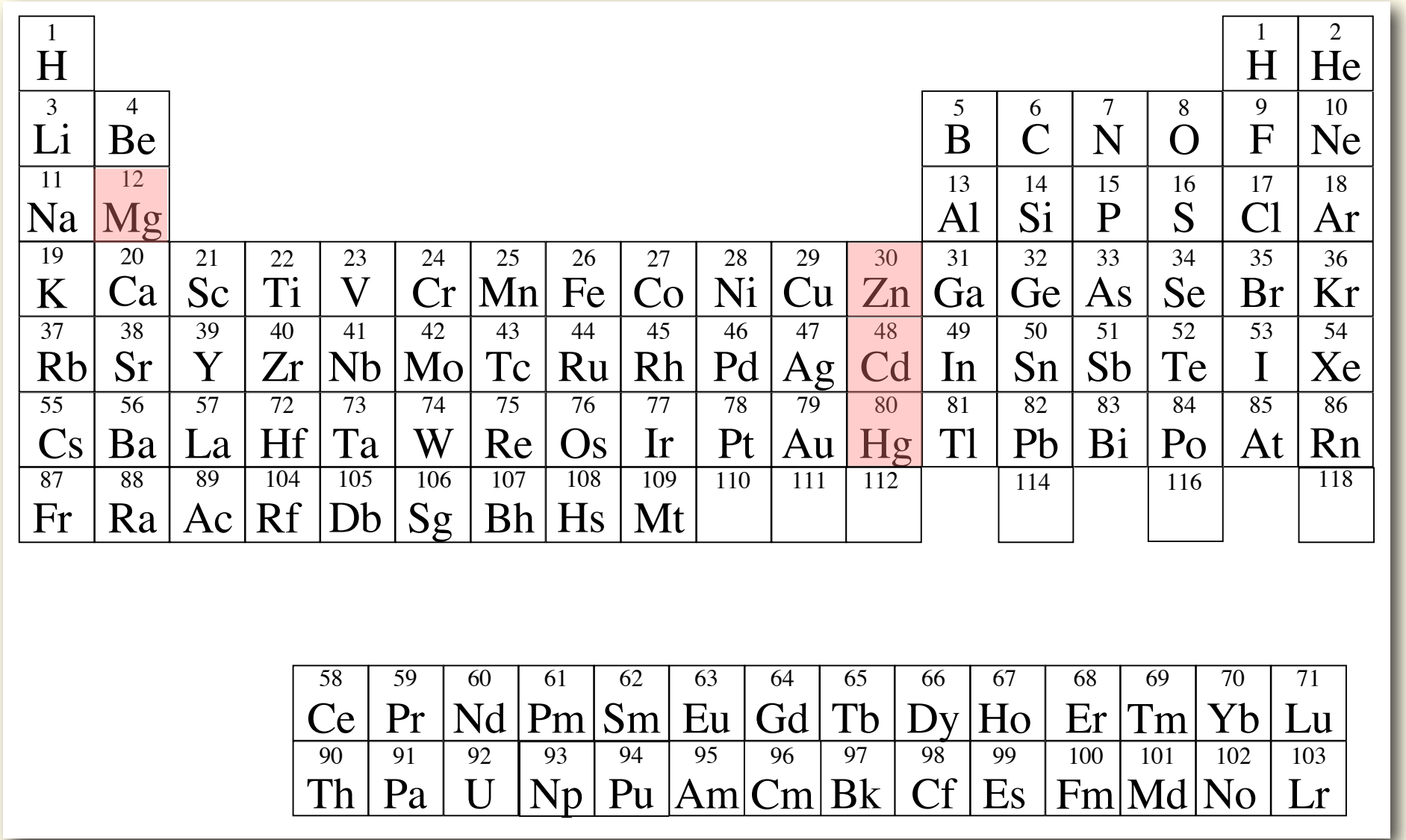
Strong attraction  BINDING

Positron-atom binding

Strong attraction → BINDING

Many-body theory calculations predicted bound states for 4 atoms

V.A. Dzuba, V.V. Flambaum, G. F. Gribakin and W.A. King, Phys. Rev. A **52**, 4541 (1995)



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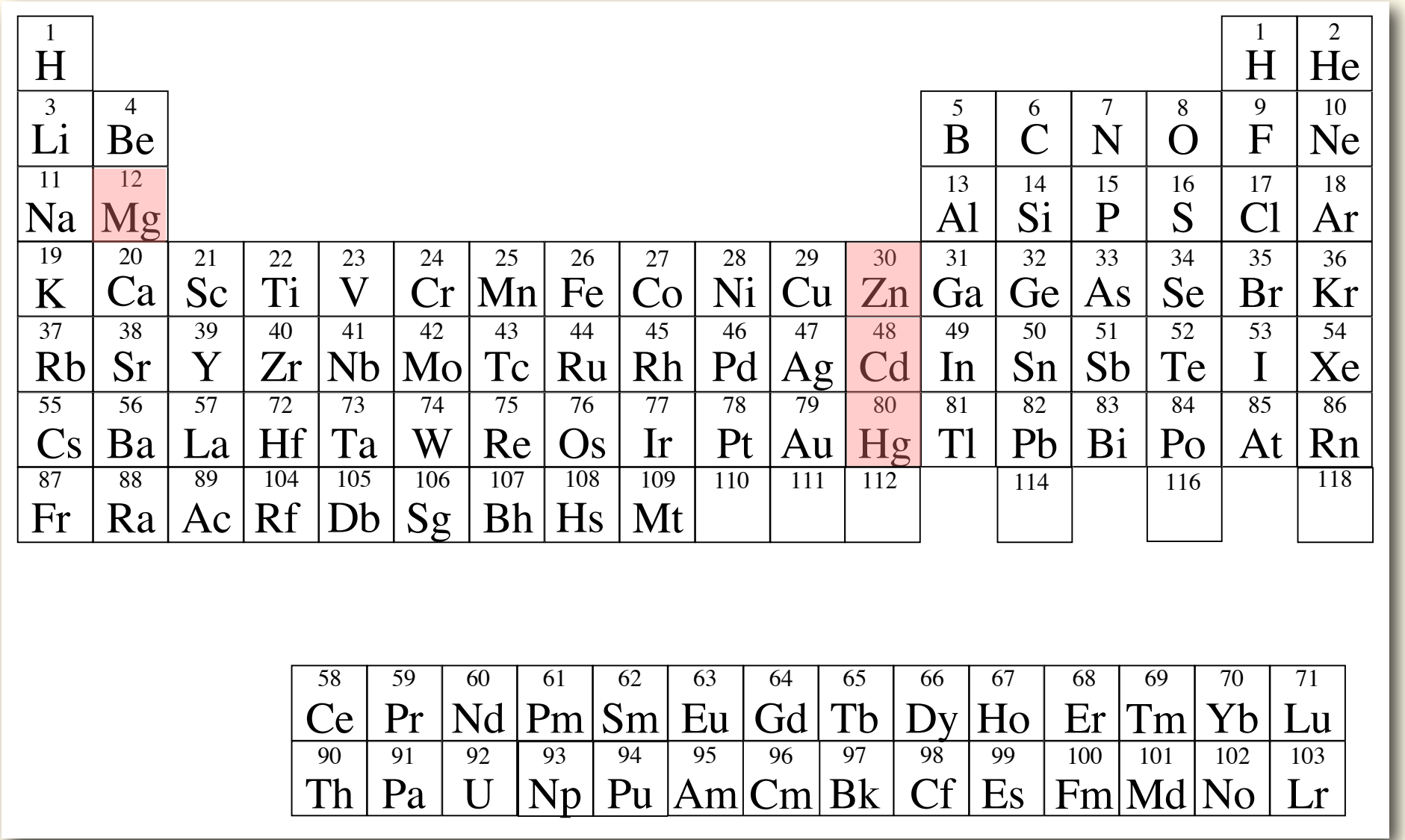

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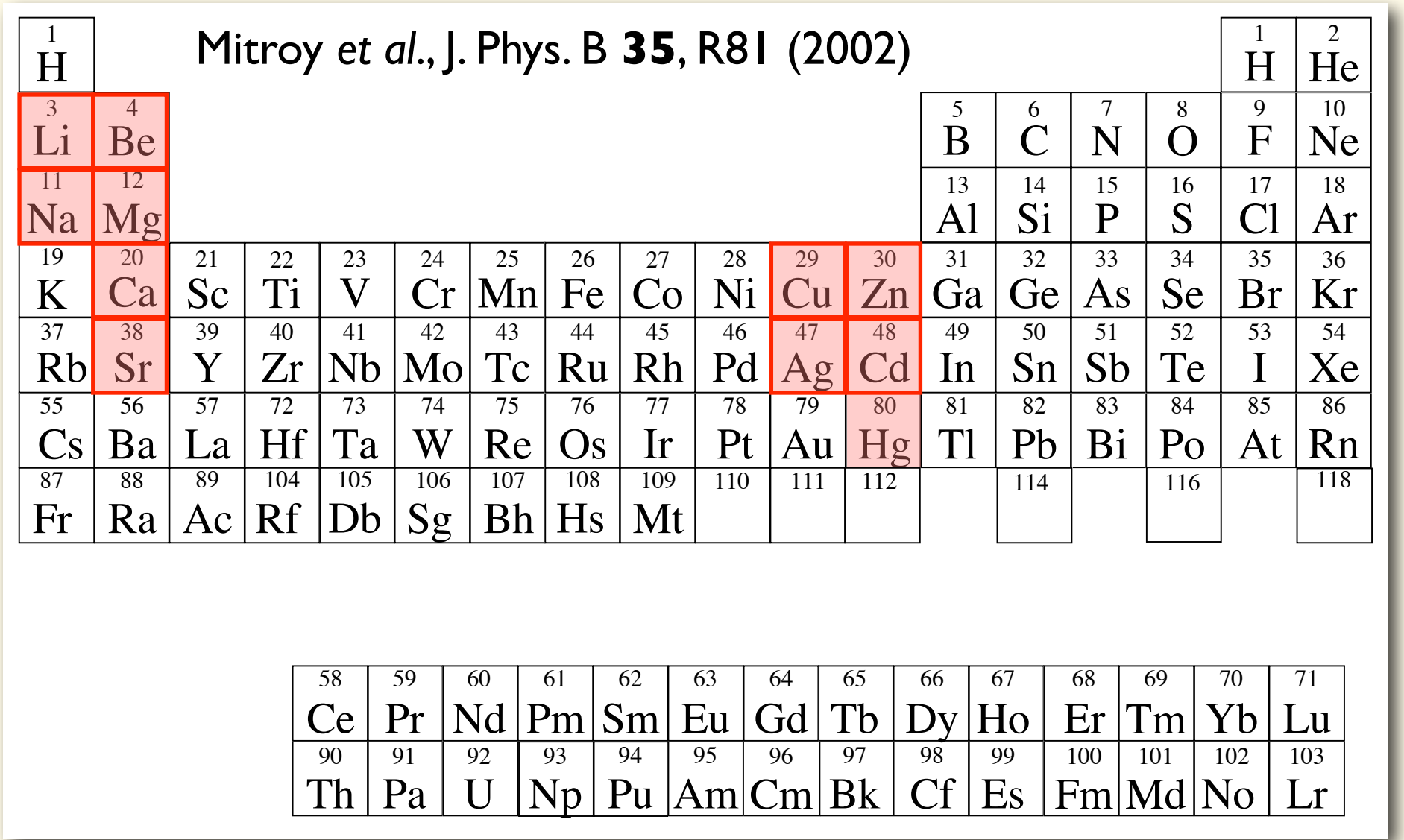
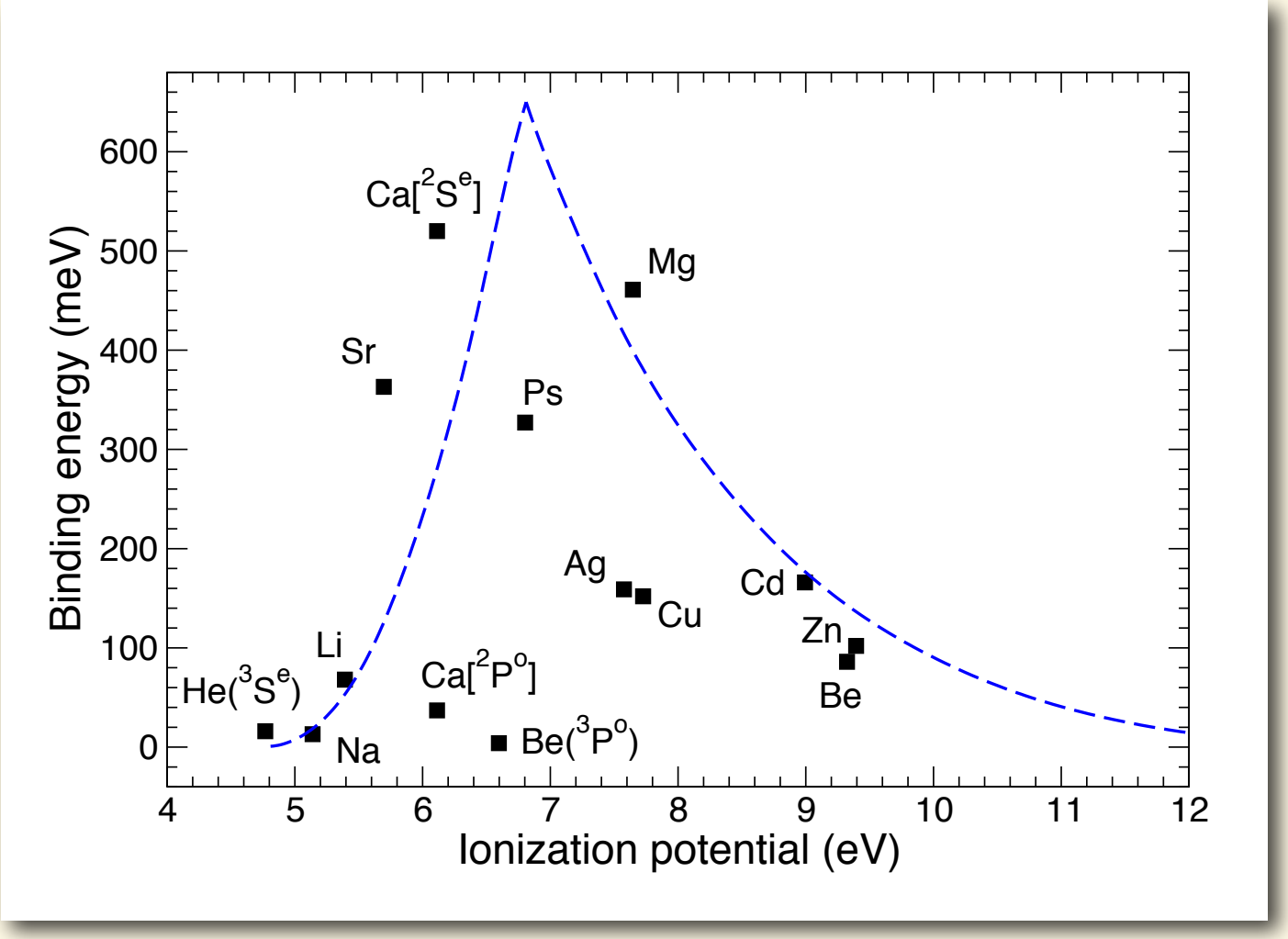


Binding by model alkali atom

J. Mitroy, M.W. J. Bromley and G. Ryzhikh, J. Phys. B **32**, 2203 (1999)



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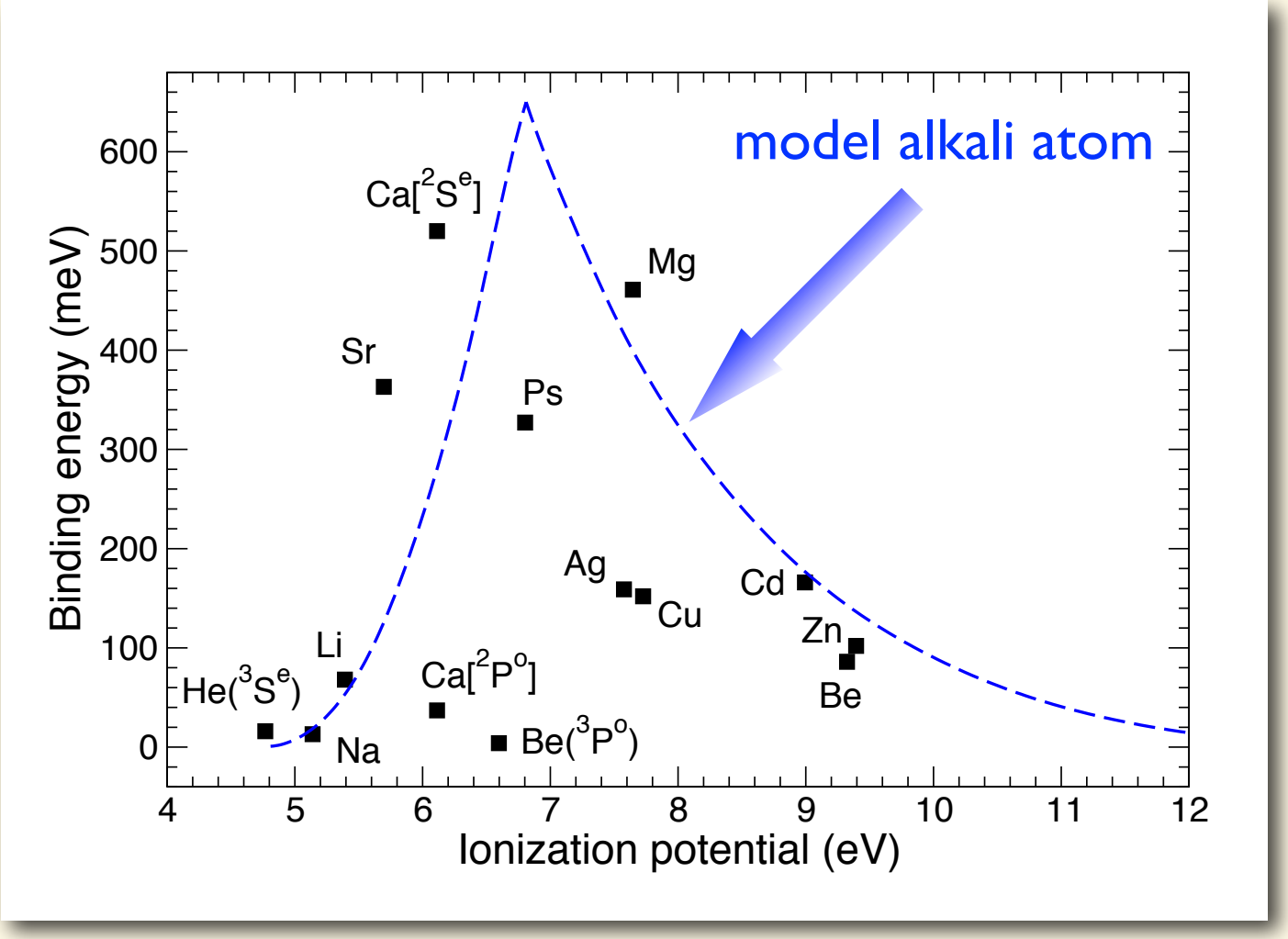

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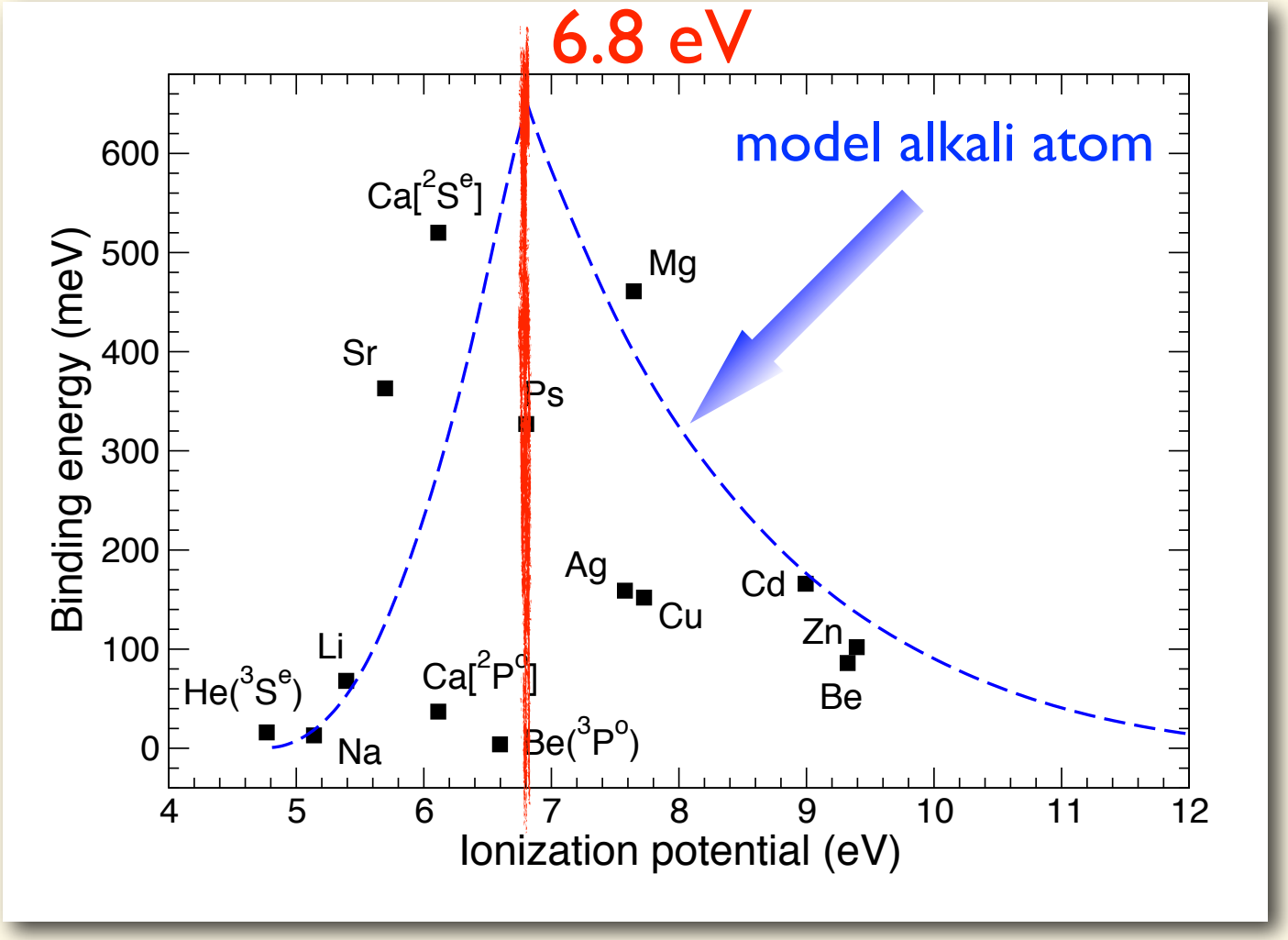

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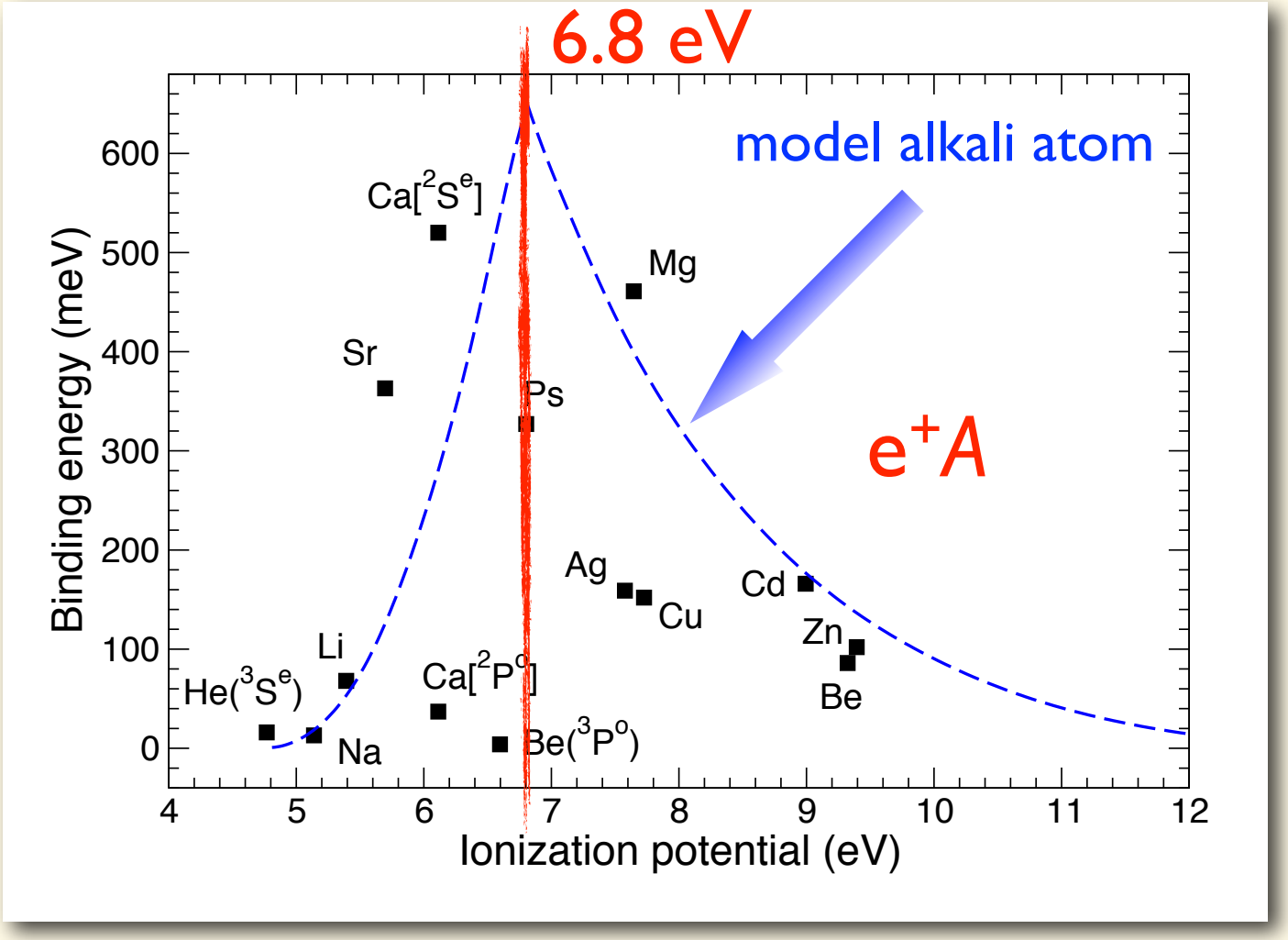

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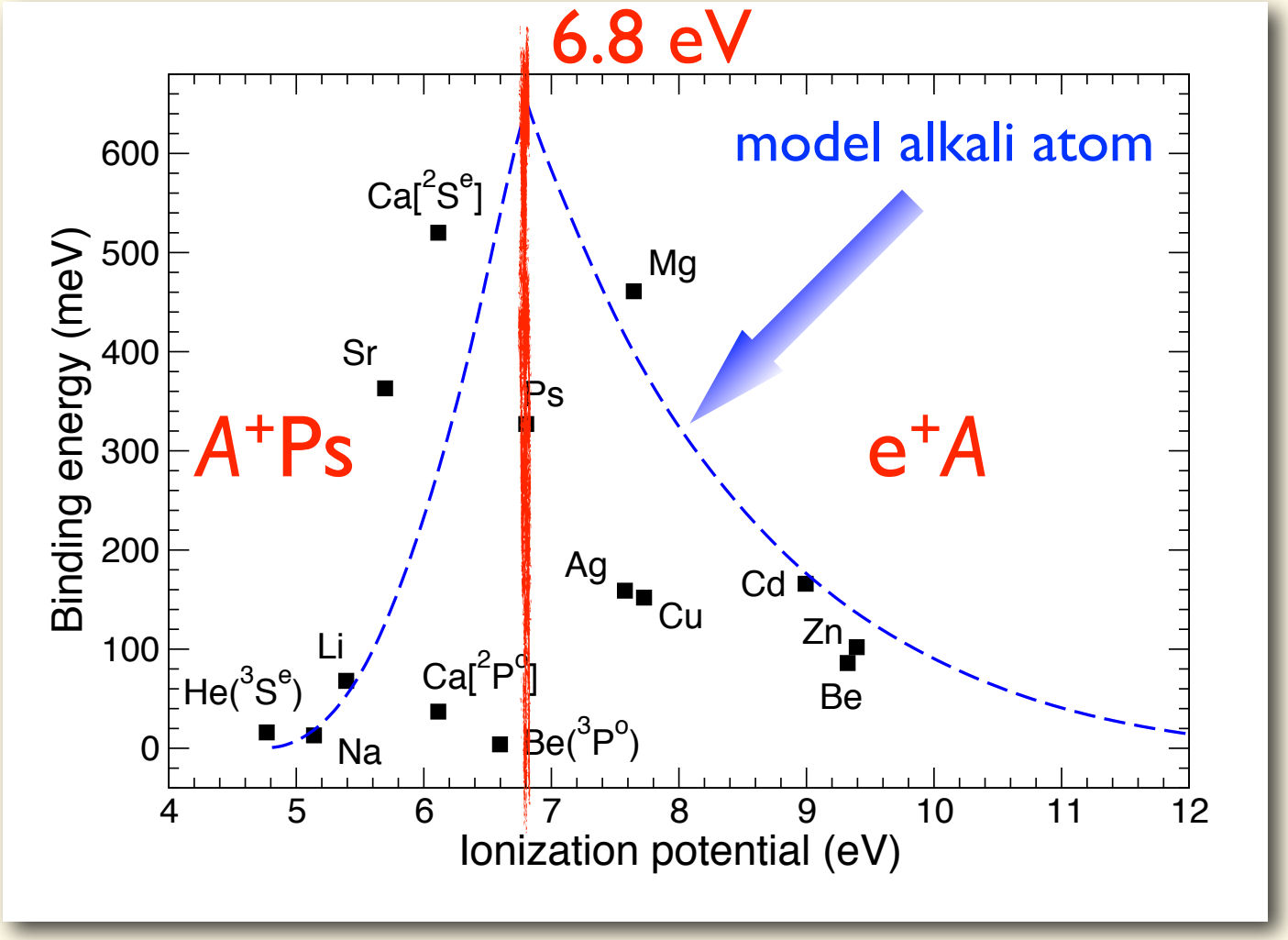

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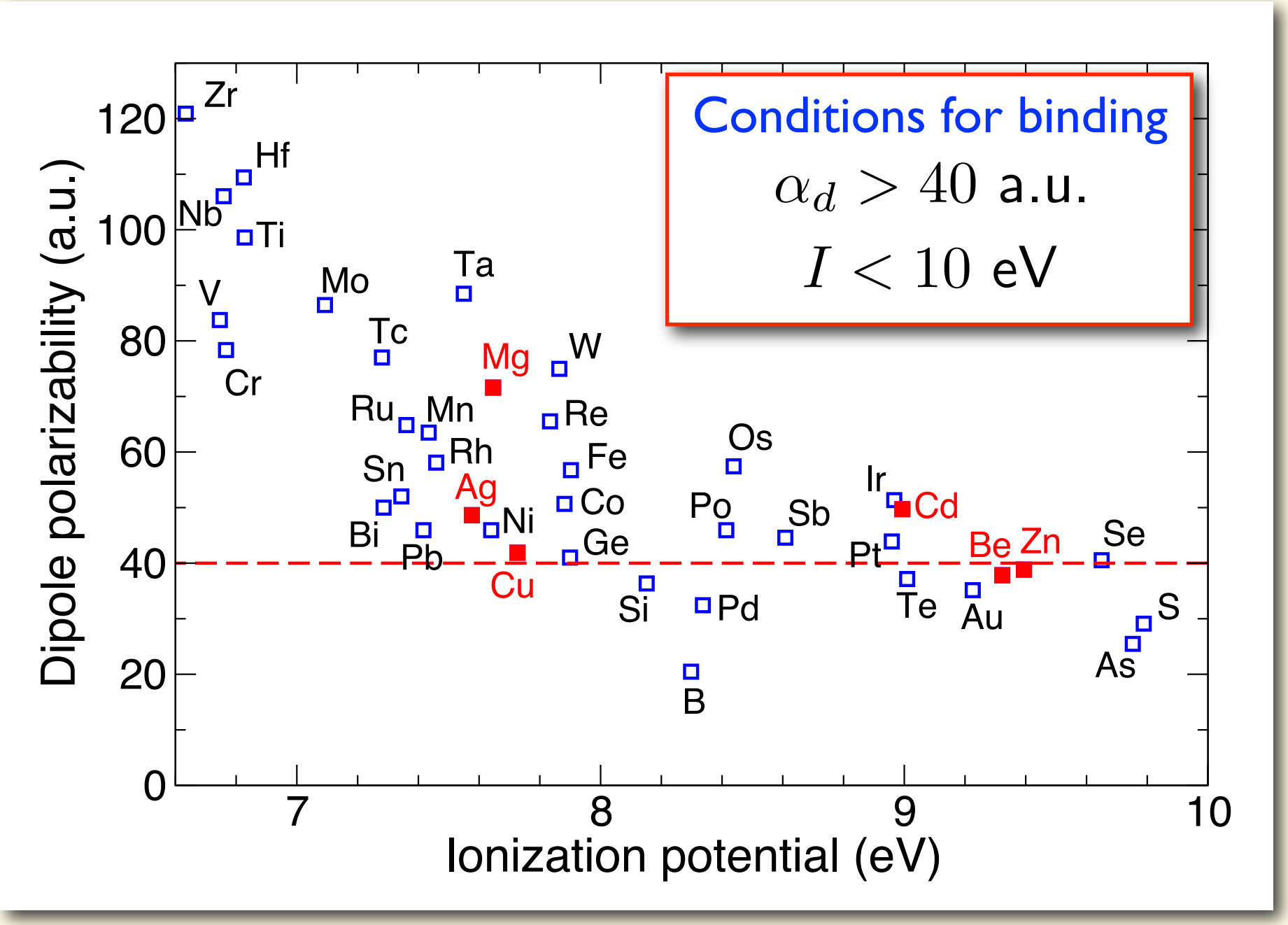
More candidates for binding

Conditions for binding

$$\alpha_d > 40 \text{ a.u.}$$

$$I < 10 \text{ eV}$$

More candidates for binding



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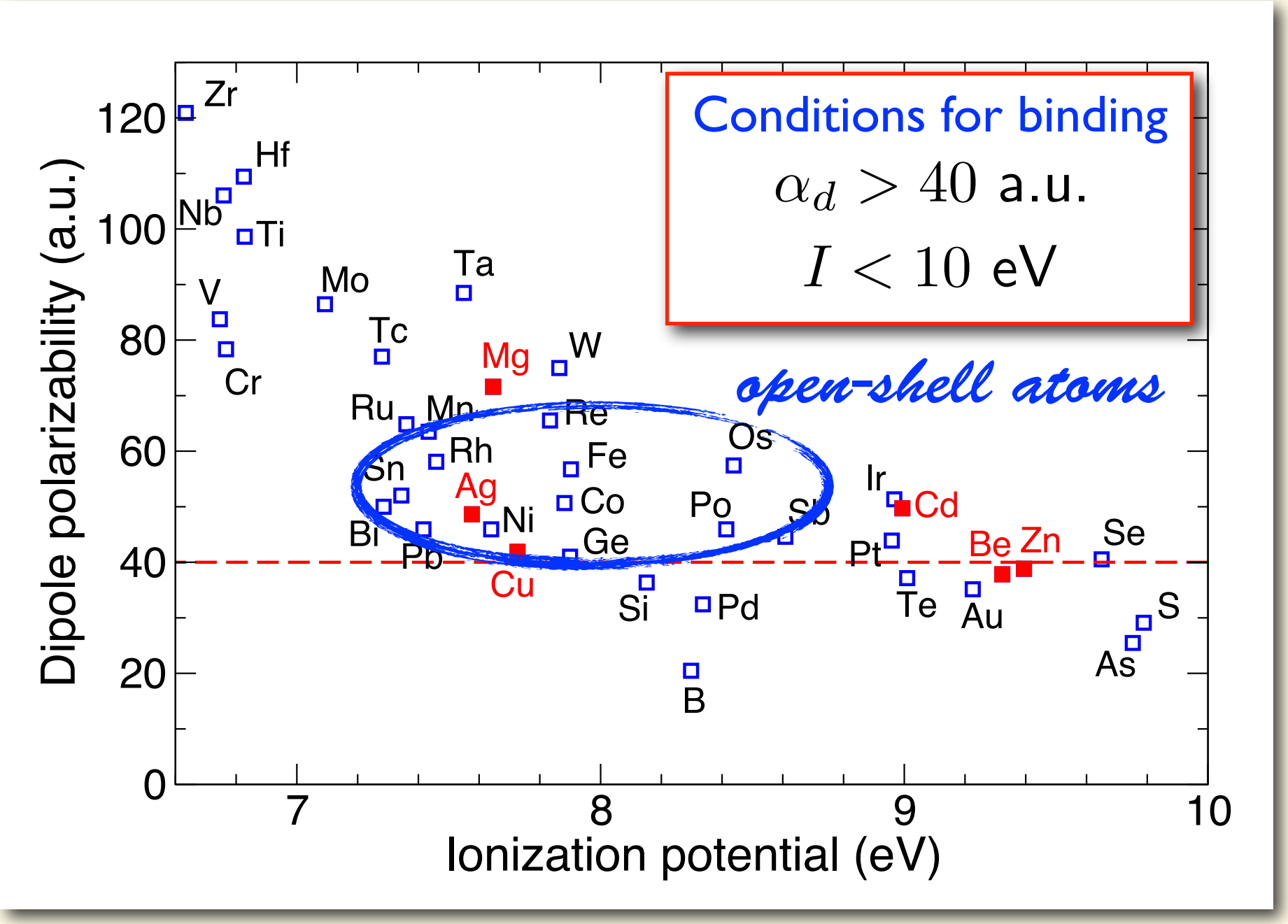

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Positron annihilation

For nonrelativitistic positrons in electronic environment

Probability of annihilation per unit time $= \underbrace{\pi r_0^2 c}_{\text{QED}} \times$ [Density of the electrons at the positron]

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$$\Gamma^a = \pi r_0^2 c \int \sum_{i=1}^{Z} \delta(\mathbf{r}_i - \mathbf{r}) |\Psi_0(\mathbf{r}_1, \ldots, \mathbf{r}_Z, \mathbf{r})|^2 d\mathbf{r}_1 \ldots d\mathbf{r}_Z d\mathbf{r}$$

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Estimate in atomic units: $c \approx 137$

$$r_0 = e^2/mc^2 \sim 10^{-4}, \quad \sigma_a \sim 10^{-6} Z_{\text{eff}}$$

Z_{eff} for atoms and small molecules

Atom	Z_{eff} *
H	8.5
He	3.94 **
Ne	5.99 **
Ar	26.8 **
Kr	65.7 **
Xe	401 ***

calc.

Molecule	Z_{eff}	Z
H_2	15	2
N_2	31	14
O_2	37	16
CO	39	14
CO_2	55	20
N_2O	78	20
SF_6	86	70
H_2O	319	18
NO_2	1090	23
NH_3	1600	10

* Values at room T, $k \sim 0.05$ au

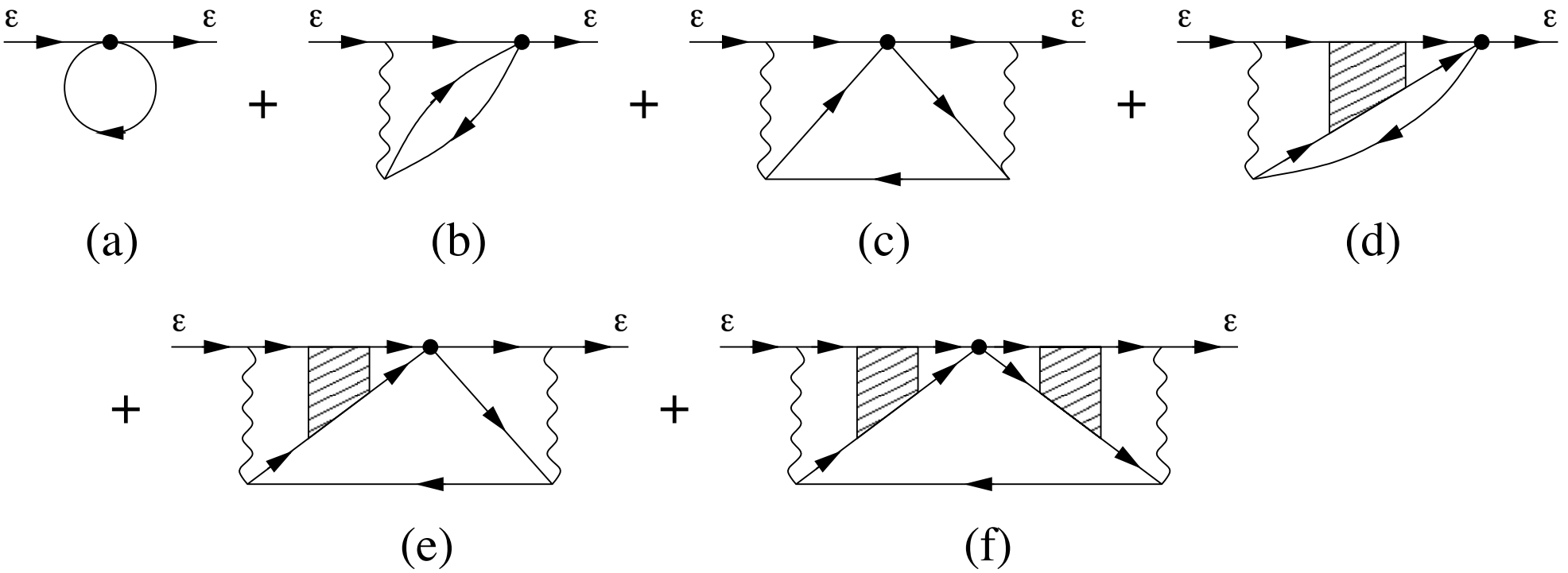
** Coleman, Charlton, Kileen, Griffith, Heyland, Wright (1975-82) (UCL)

*** Iwata *et al.* (1995) (UCSD)

Positron annihilation: many-body theory

$$Z_{\rm eff} = \int \sum_{i=1}^{Z} \delta(\mathbf{r}_i - \mathbf{r}) |\Psi_{\mathbf{k}}(\mathbf{r}_1, \ldots, \mathbf{r}_Z, \mathbf{r})|^2 d\mathbf{r}_1 \ldots d\mathbf{r}_Z d\mathbf{r}$$

Annihilation vertex and corrections



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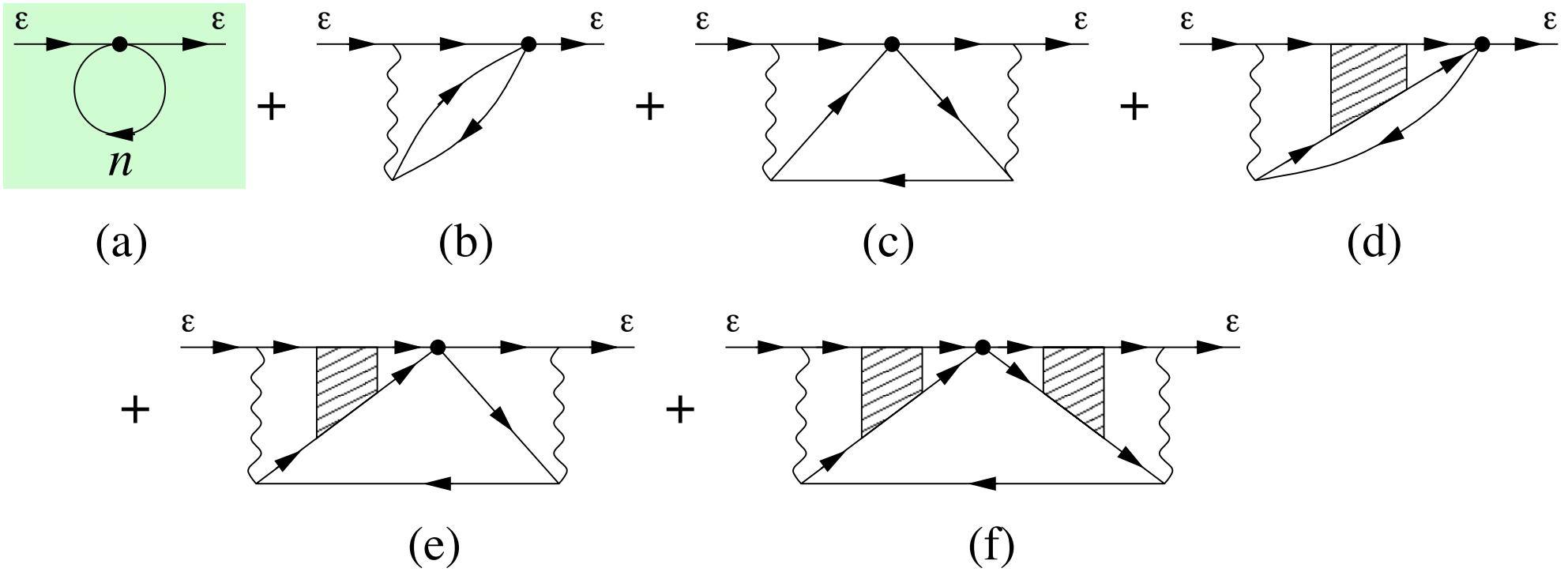

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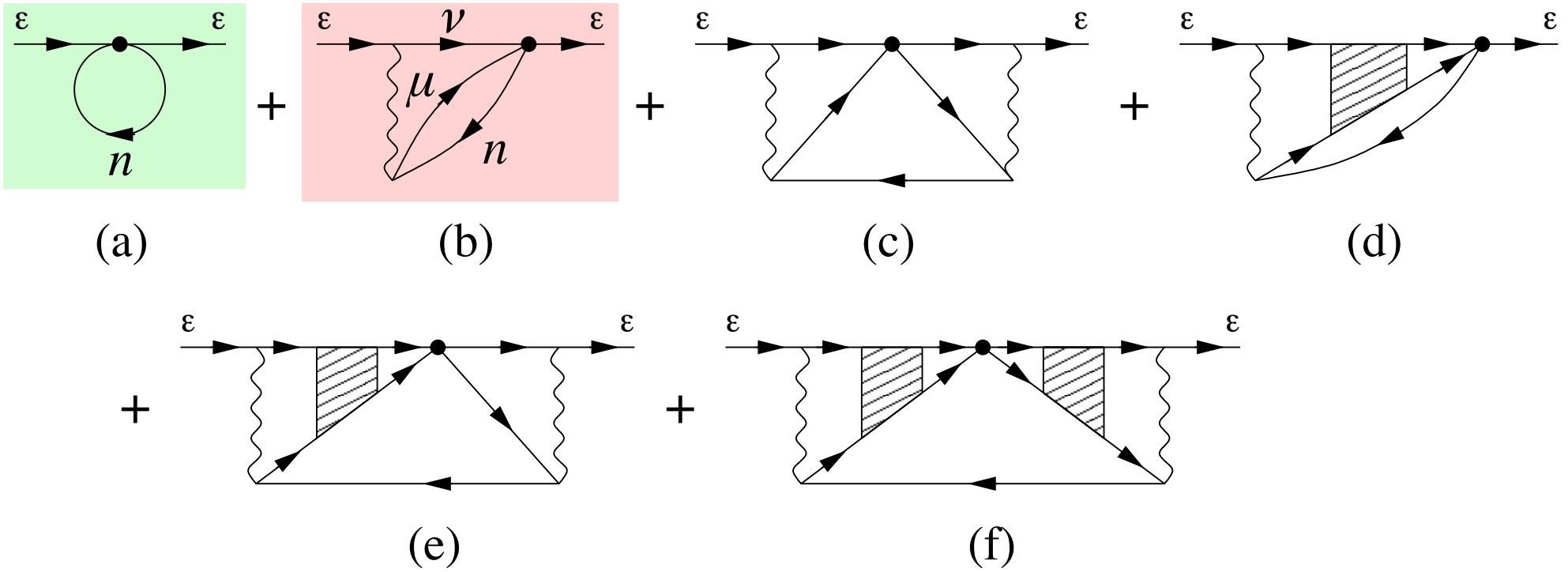

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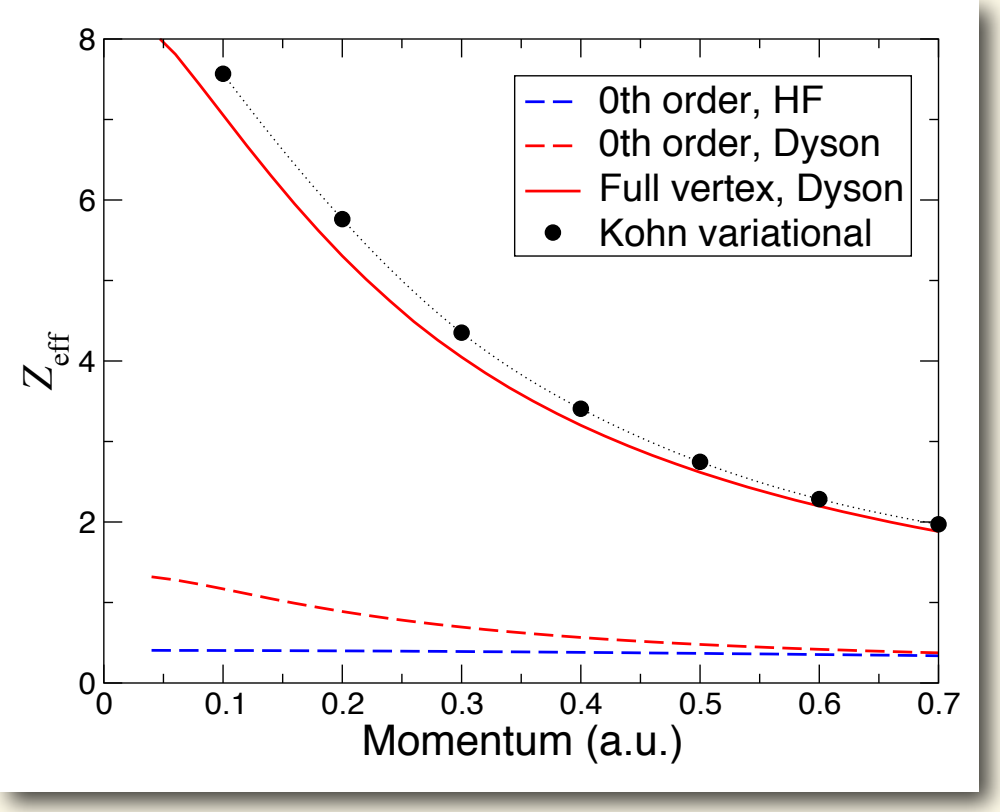
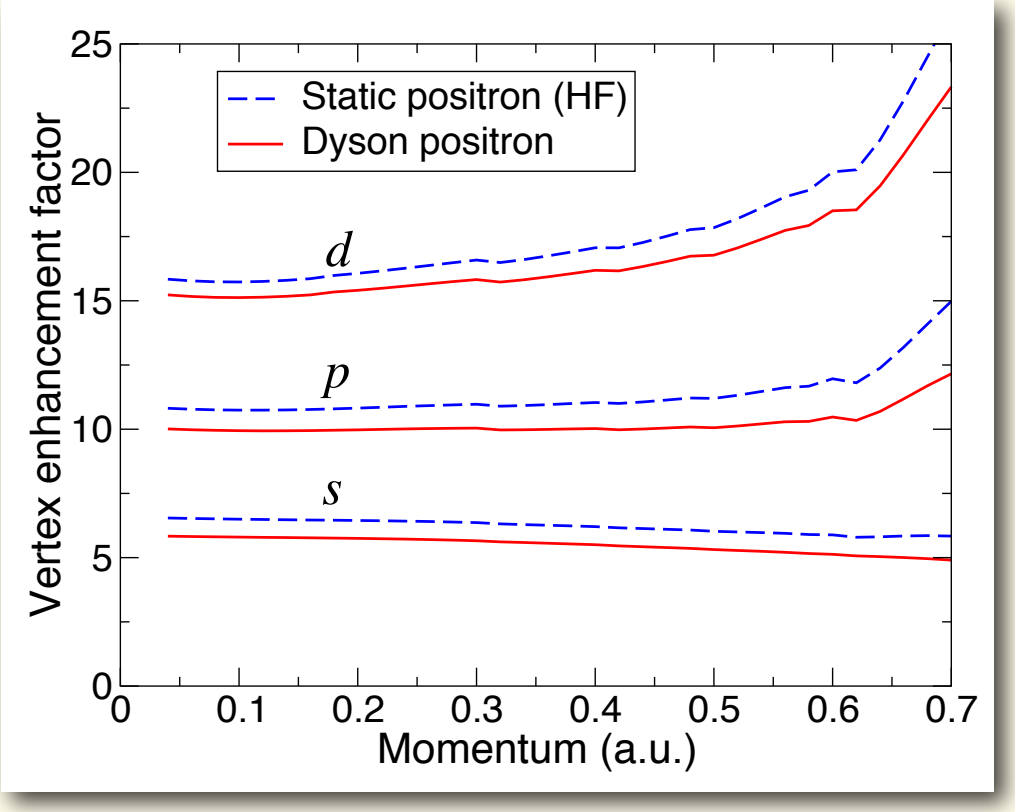
$$Z^{(1)}_{\rm eff} = \sum_{\nu,\,\mu,\,n} \frac{\langle \varepsilon n|\delta|\mu\nu\rangle\langle\nu\mu|V|n\varepsilon\rangle}{\varepsilon - \varepsilon_\nu - \varepsilon_\mu + \varepsilon_n}$$

Z_{eff} for hydrogen





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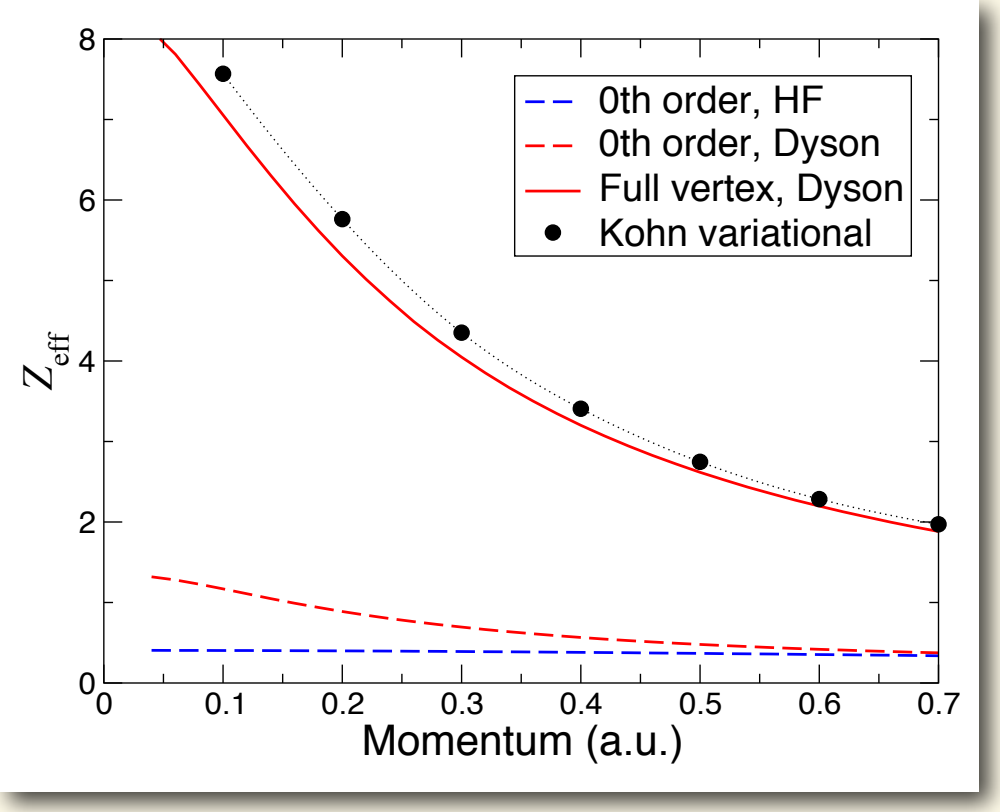

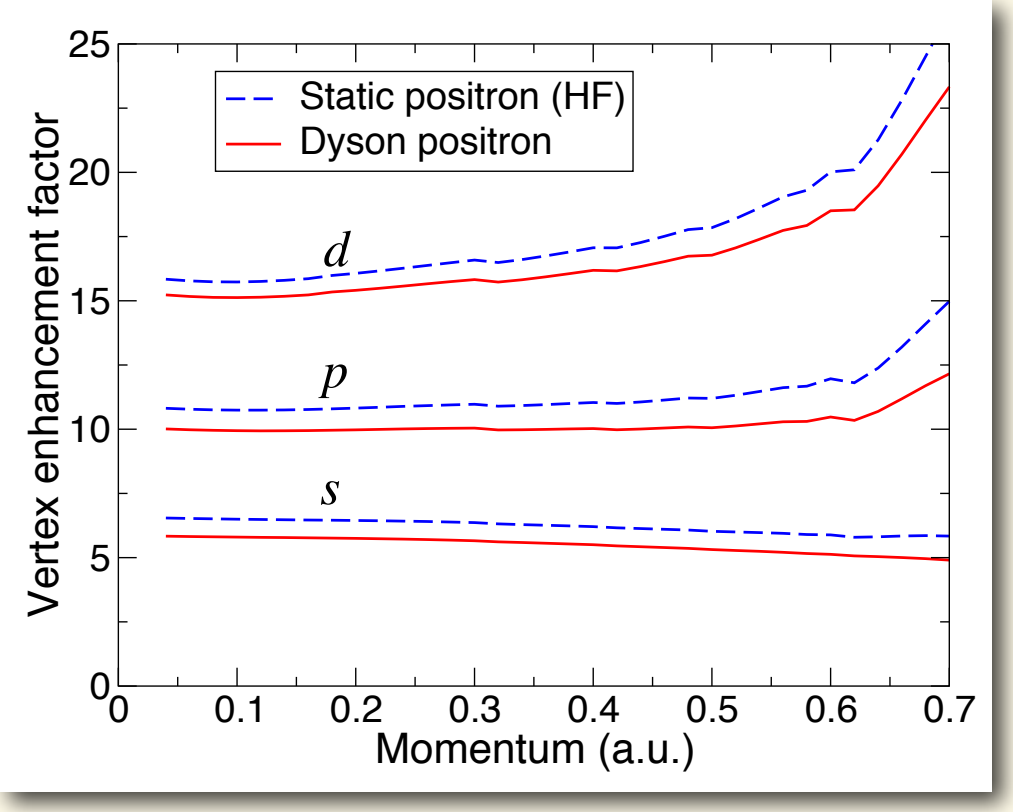

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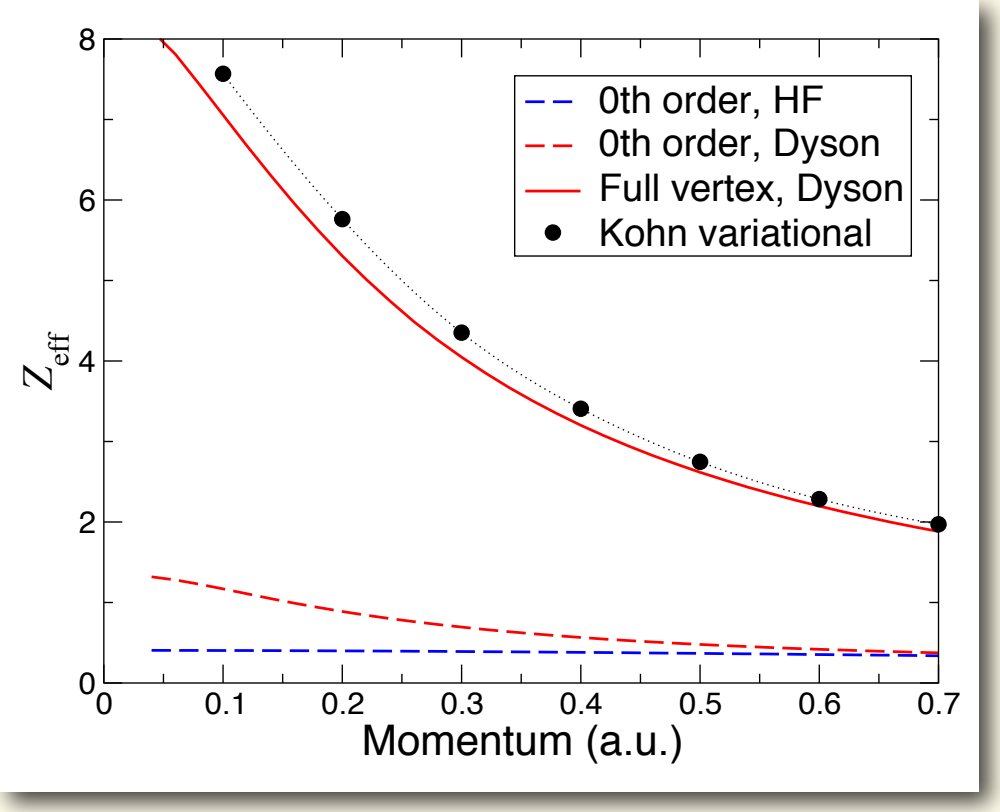

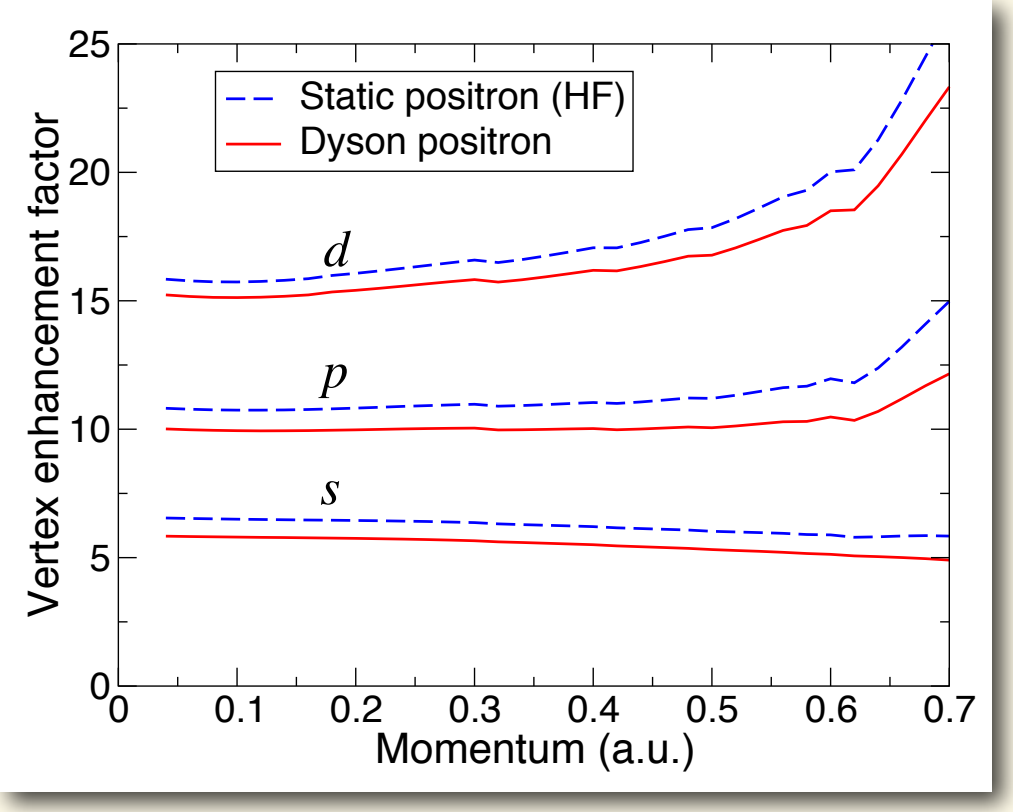

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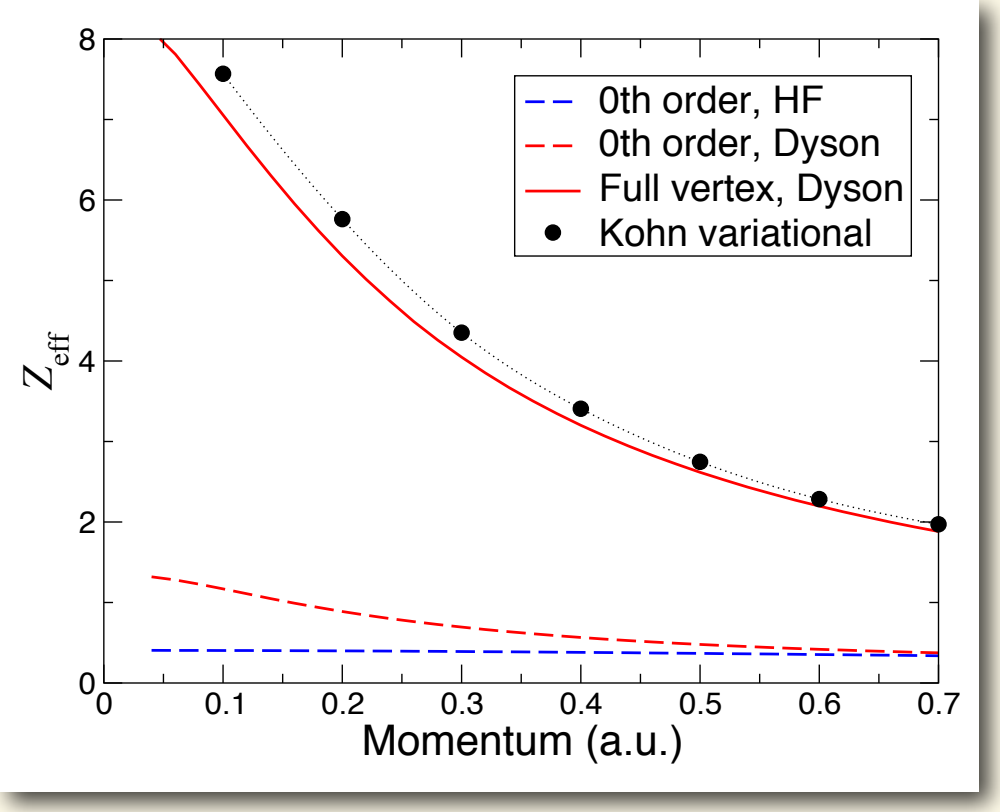
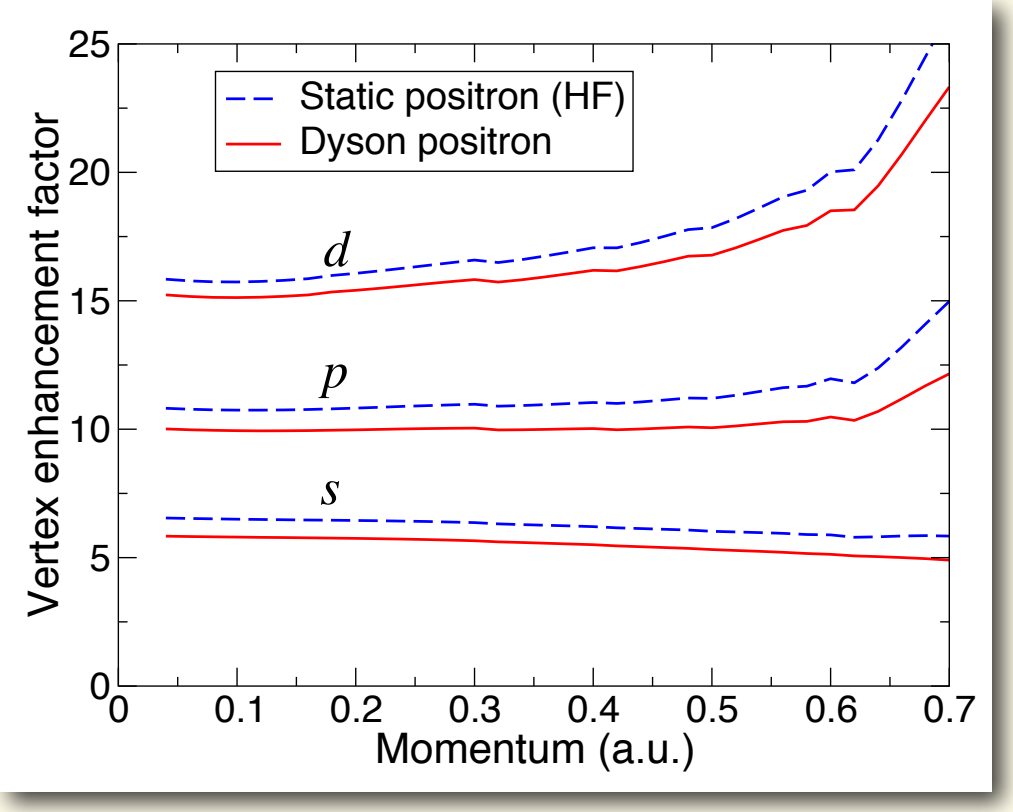
Scattering amplitude

Z_{eff} for hydrogen





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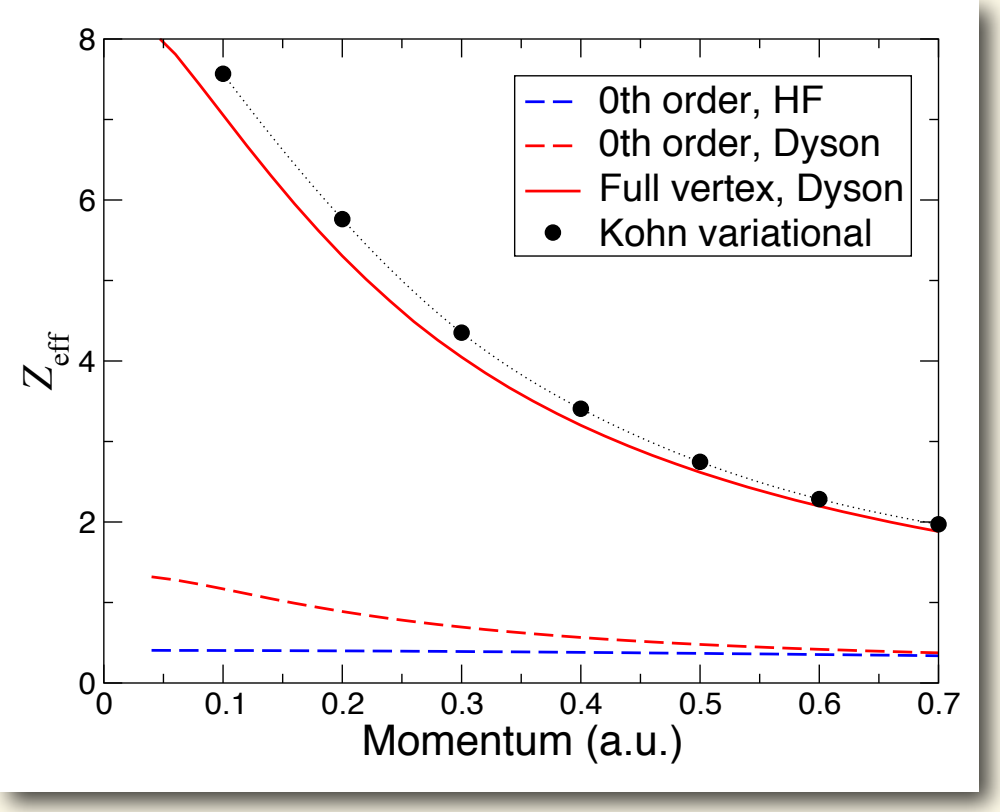

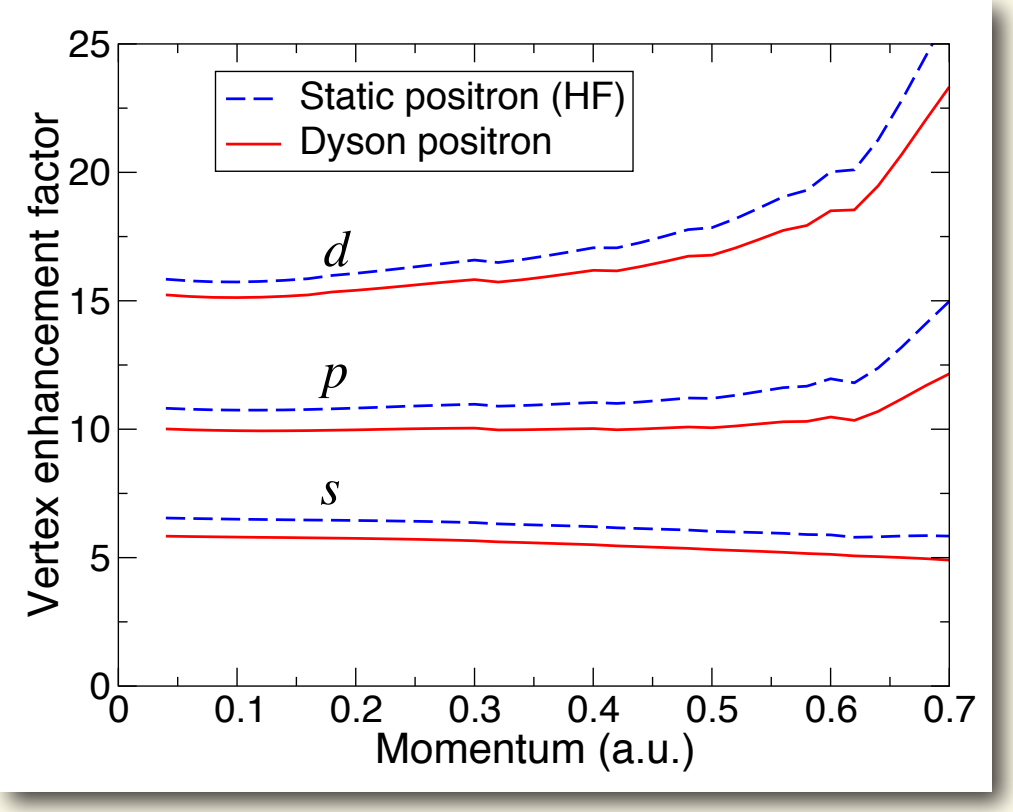

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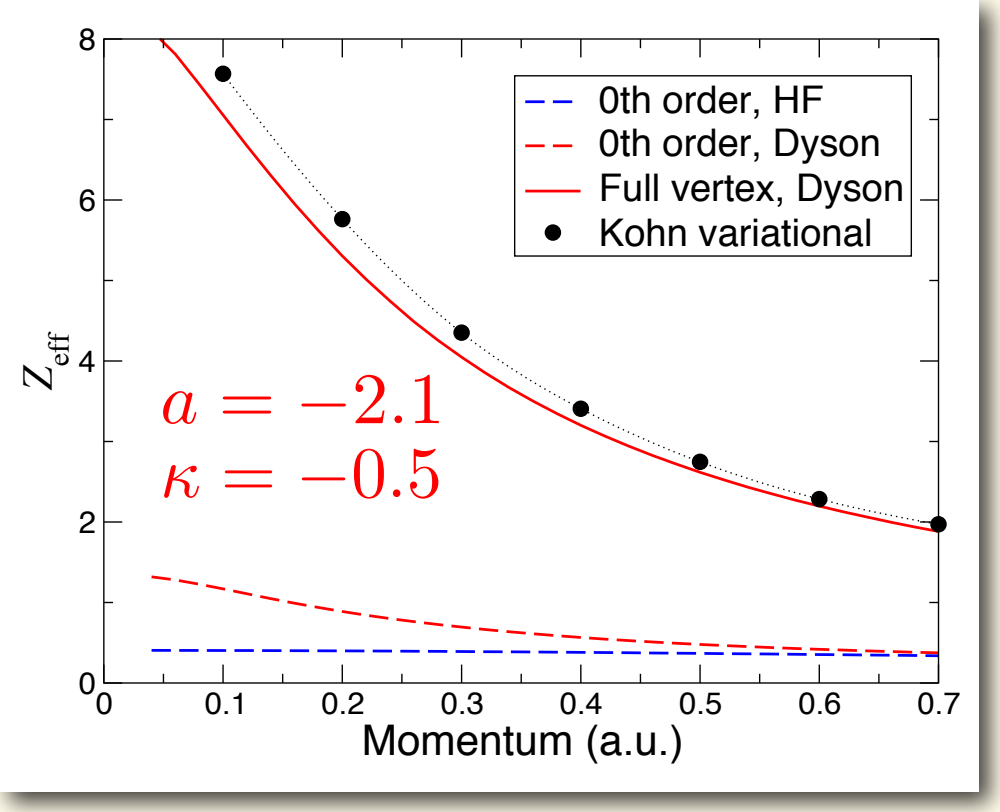

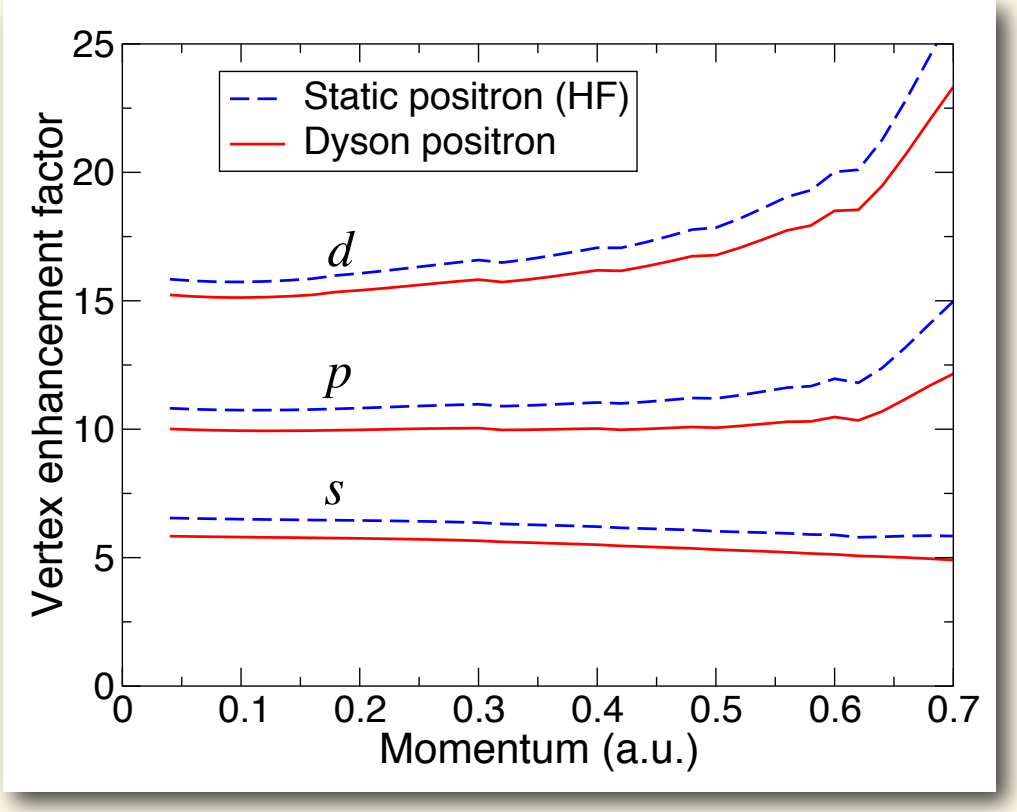

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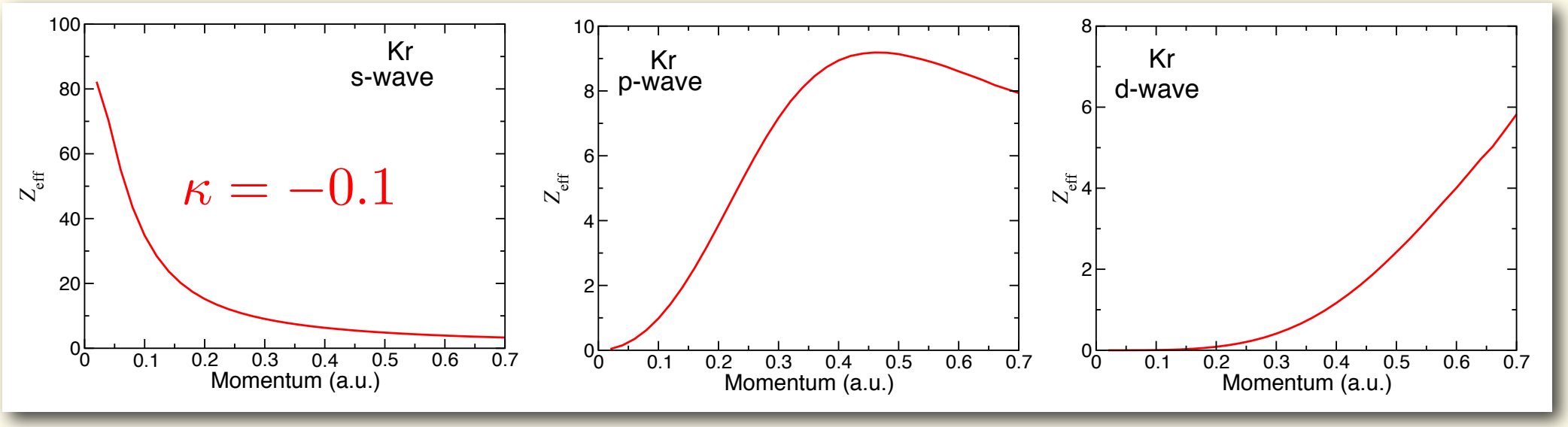
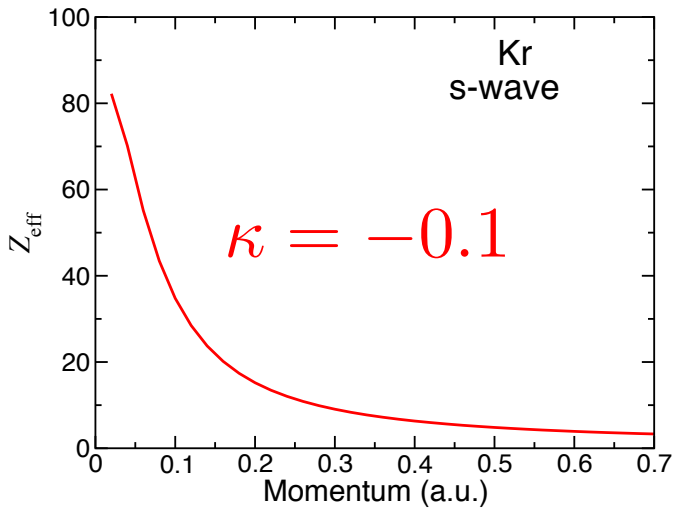
Annihilation on noble gases

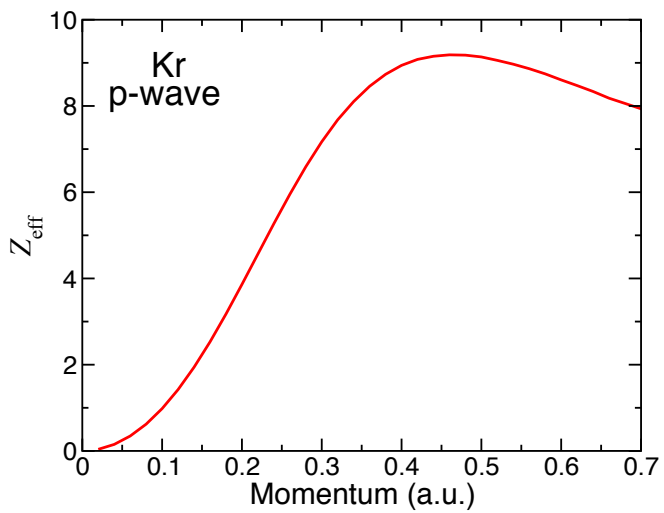
Krypton

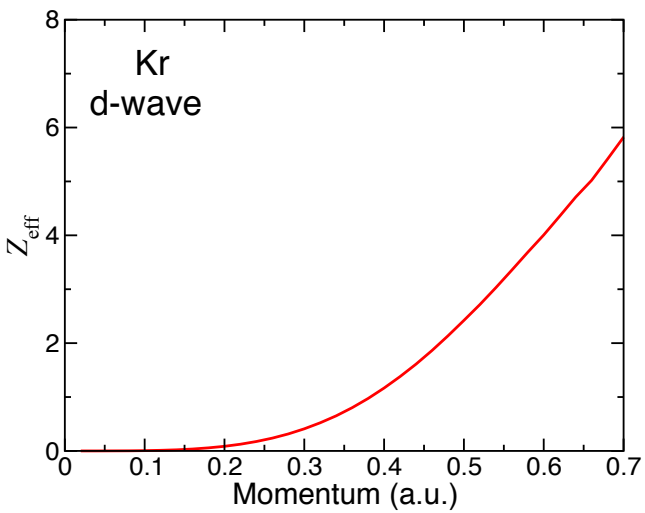


Annihilation on noble gases

Krypton







Thermally averaged $Z_{\rm eff}$ at room T

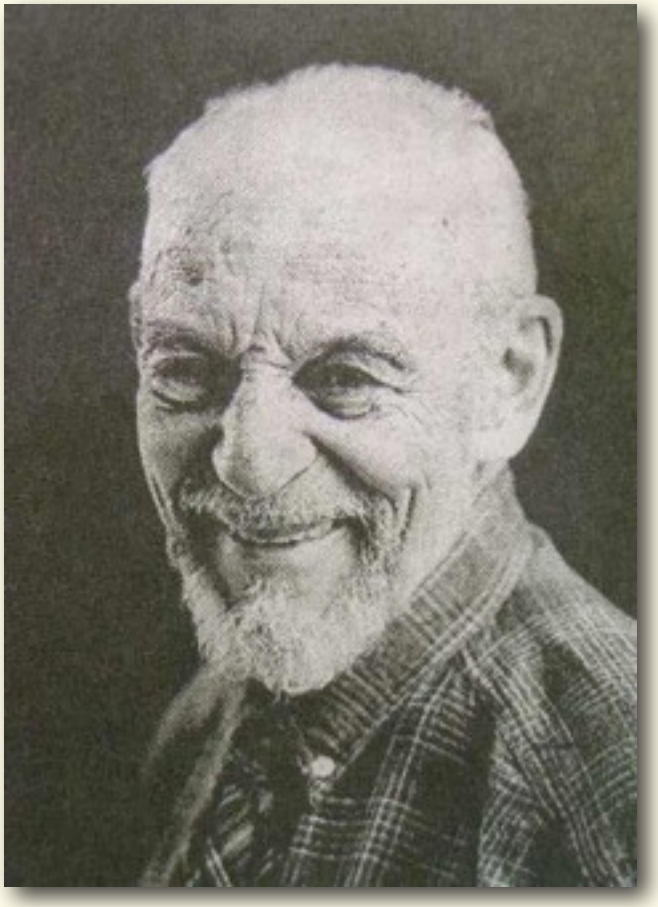
Atom	He	Ne	Ar	Kr	Xe
0th order, static	0.69	0.97	0.74	0.68	0.61
0th order, Dyson	1.34	2.30	6.86	14.6	71
total, Dyson	3.78	5.53	26.5	66.4	402
Exp. (gas)	3.94	5.99	26.8	65.7	320
Exp. (trap, UCSD)	-	-	33.8	90.1	401

Positron annihilation in molecules

Martin Deutsch (1917-2002)

- Discovery of Ps (1951)
- Measurement of lifetime of Ps
- Single-triplet Ps energy splitting

Rapid annihilation of positrons in Freon-12, CCl_2F_2



The Times 22 October 2002

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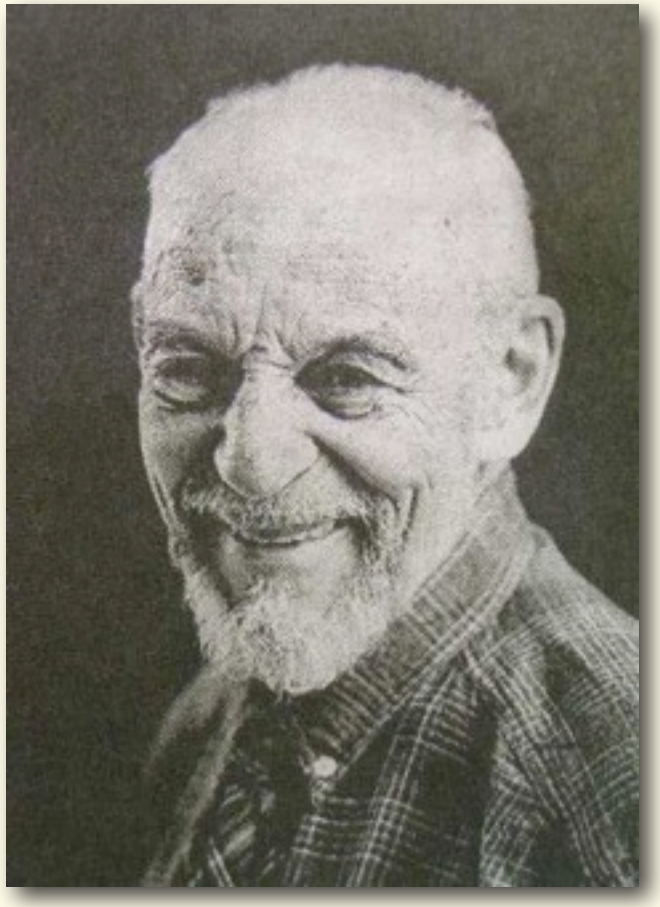

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Paul & Saint-Pierre (1963): $Z_{\mathrm{eff}} \sim 10^4$ for C_4H_{10} and CCl_4

Tao (1965): $Z_{\mathrm{eff}} \sim 1600$ for Cl_2 (UNSW)

Heyland *et al.* (1982), Wright *et al.* (1985): C_3H_8 , …

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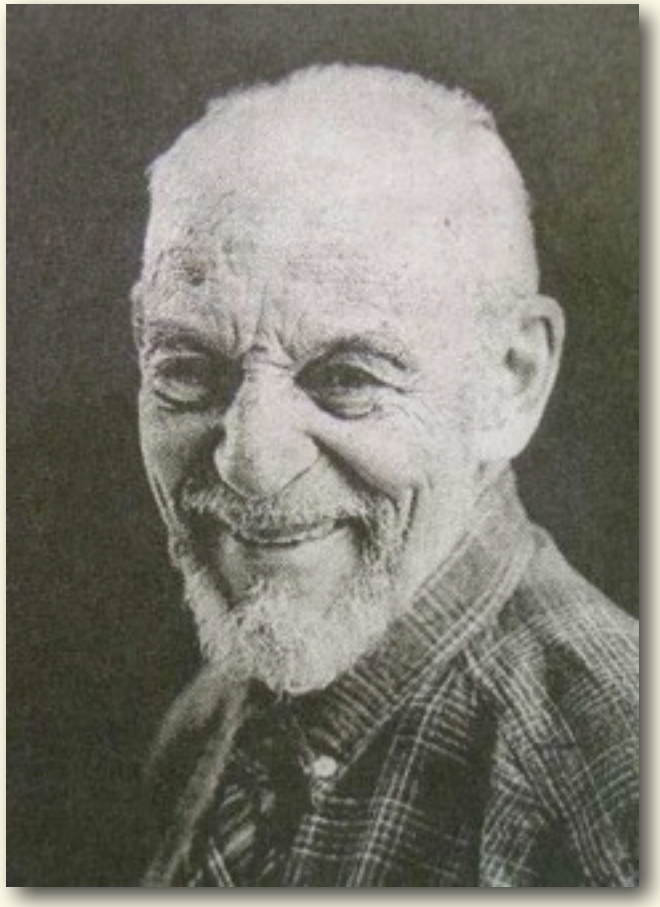
For room-temperature positrons

$$Z_{\rm eff} = \frac{F}{\kappa^2 + k^2} \lesssim 10^3$$



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Z_{eff} for alkanes and substitutes

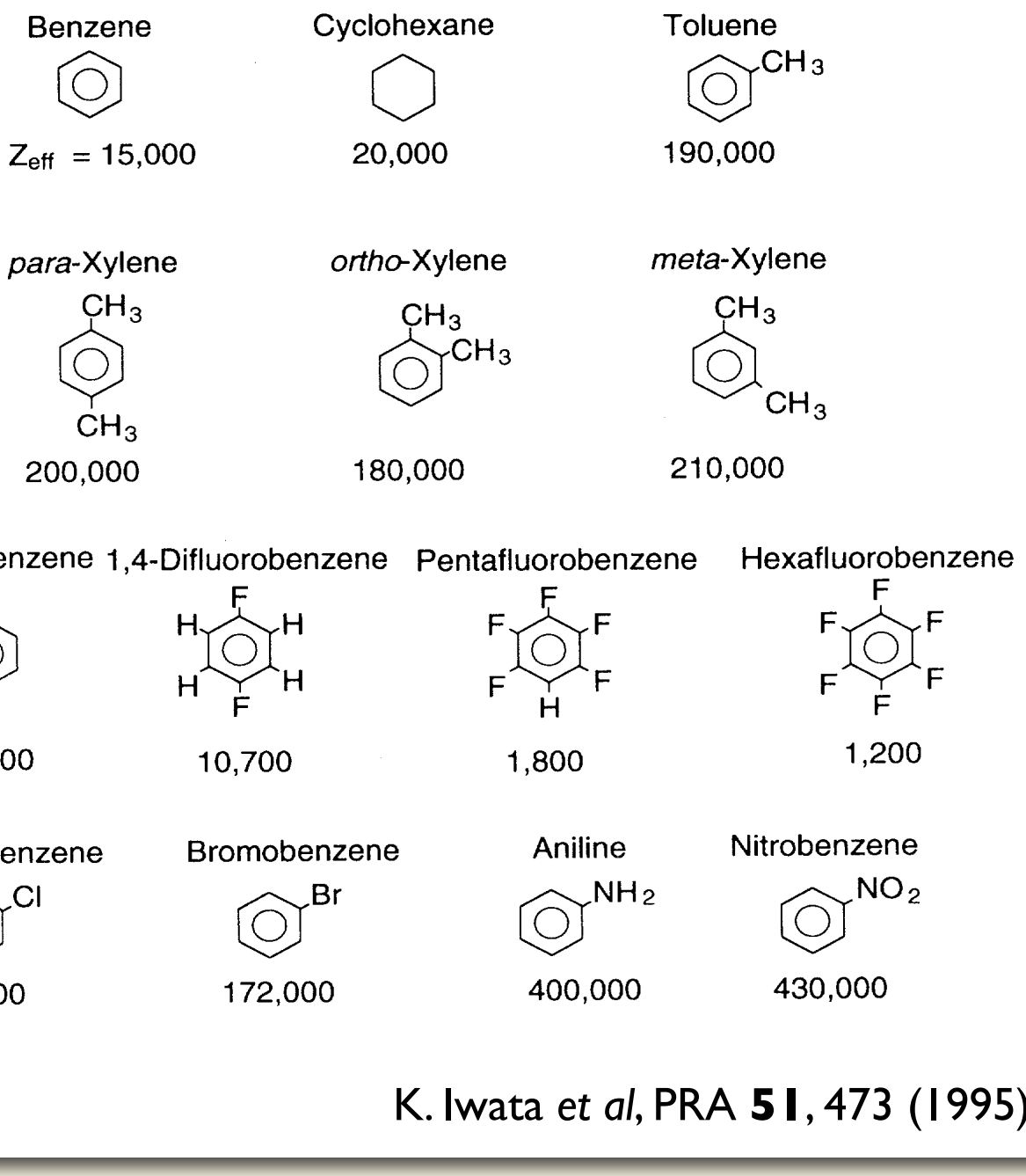
Molecule	Z_{eff}	Z
H_2	15	2
N_2	31	14
O_2	37	16
CO	39	14
CO_2	55	20
N_2O	78	20
SF_6	86	70
H_2O	319	18
NO_2	1090	23
NH_3	1600	10

Z_{eff} for alkanes and substitutes

Molecule	X = H	X = F	X = Cl	X = Br
CX_4	142	54.4	9 530	39 800
C_2X_6	660	152	68 600	-
C_3X_8	3 500	317	-	-
C_4X_{10}	11 300	-	-	-
C_5X_{12}	37 800	-	-	-
C_6X_{14}	120 000	630	-	-
C_7X_{16}	242 000	-	-	-
C_8X_{18}	585 000	1 064	-	-
C_9X_{20}	643 000	-	-	-
$C_{10}X_{22}$	728 000	-	-	-
$C_{12}X_{26}$	1 780 000	-	-	-
$C_{16}X_{34}$	2 230 000	-	-	-

Iwata, Greaves, Murphy, Tinkle and Surko, PRA **51**, 473 (1995)

Chemical sensitivity of Z_{eff}



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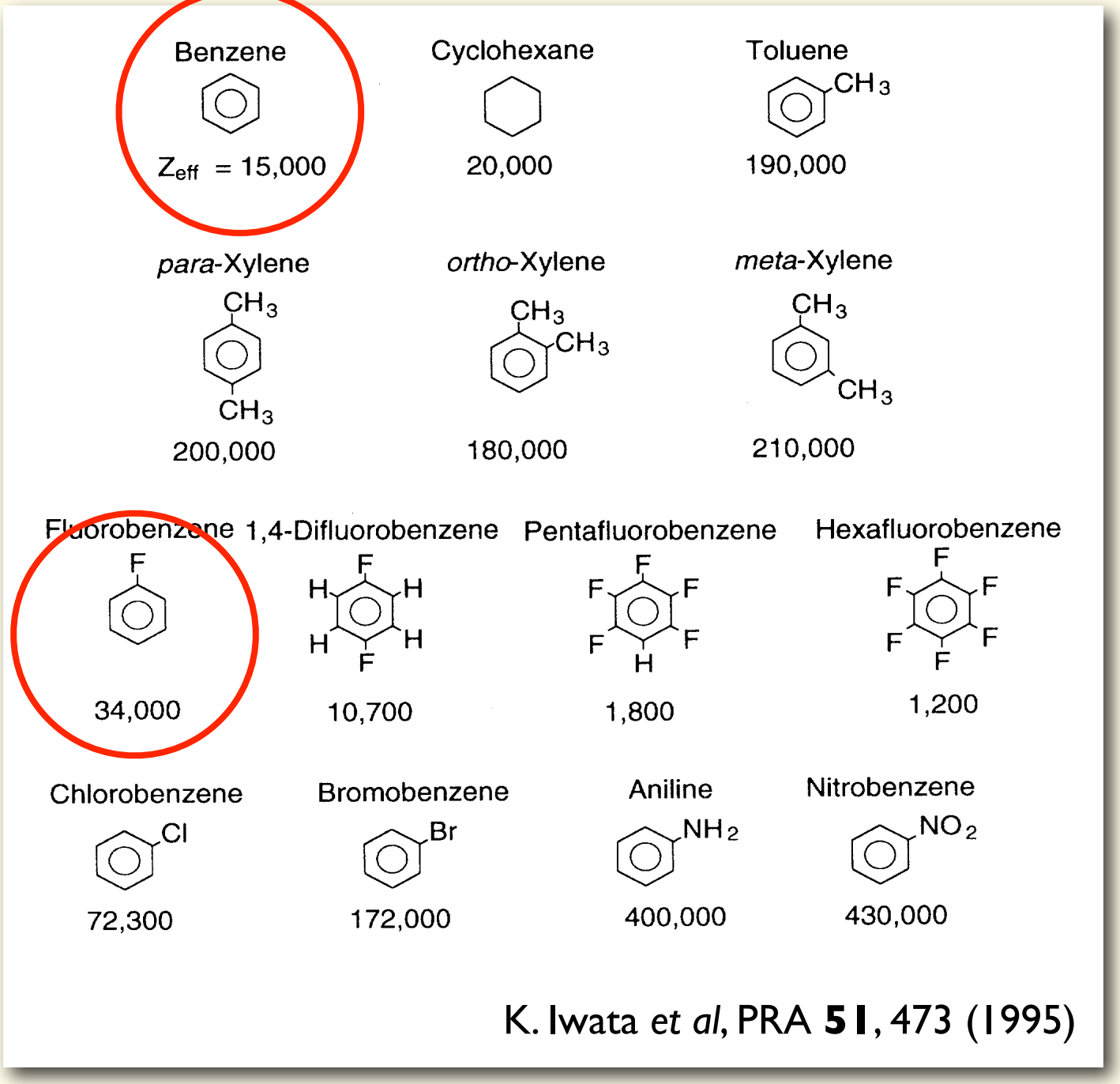

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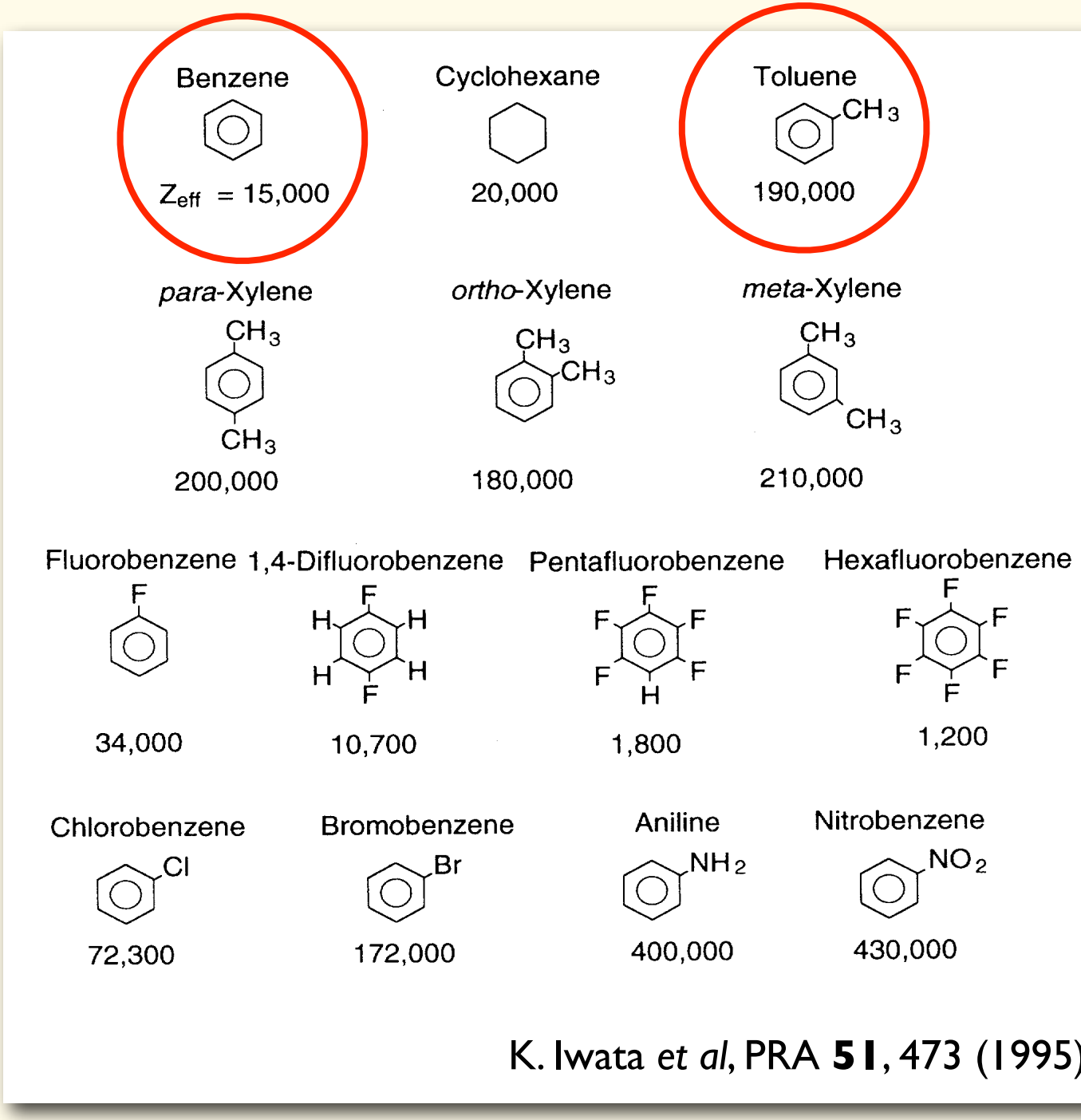

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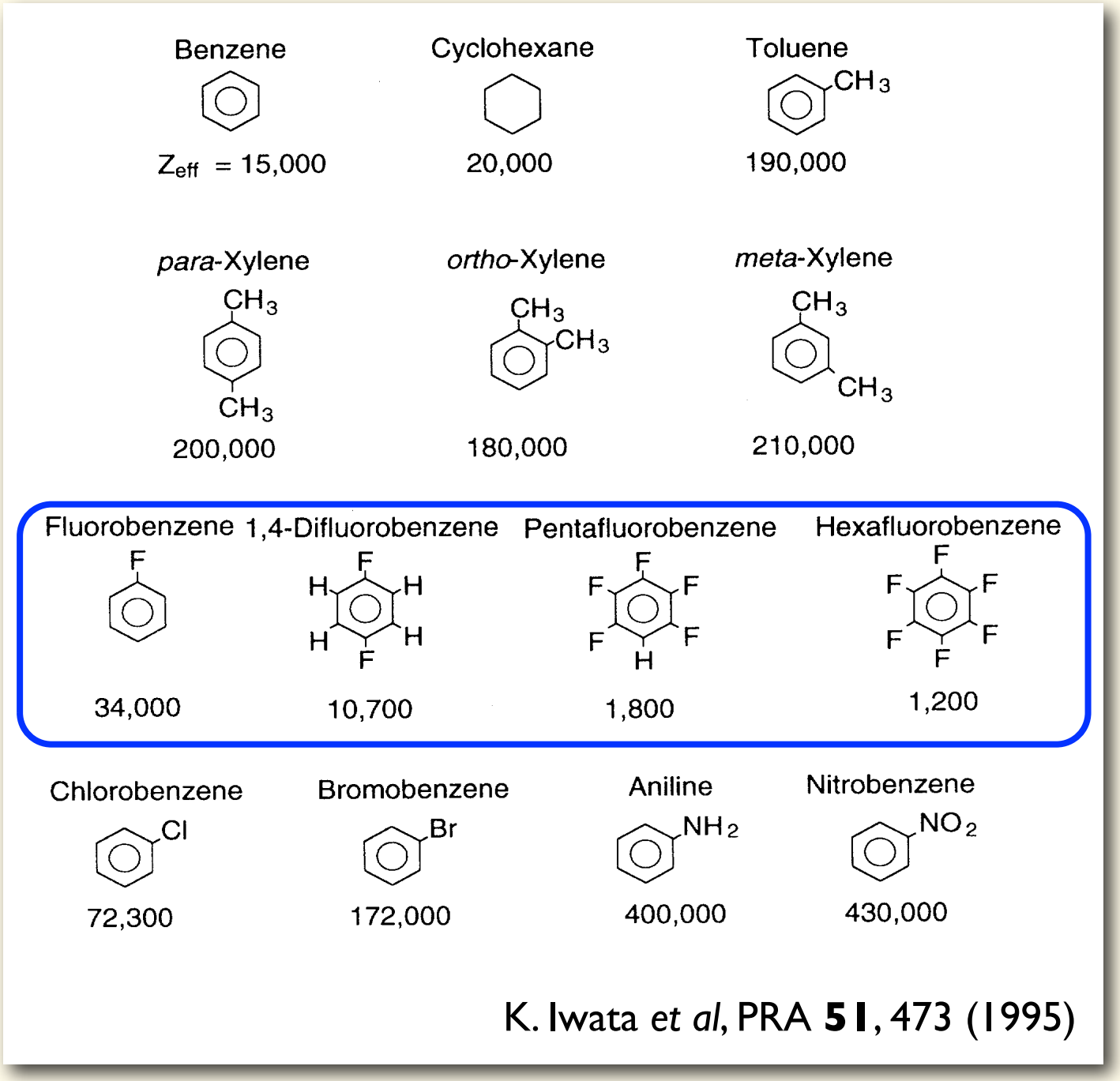

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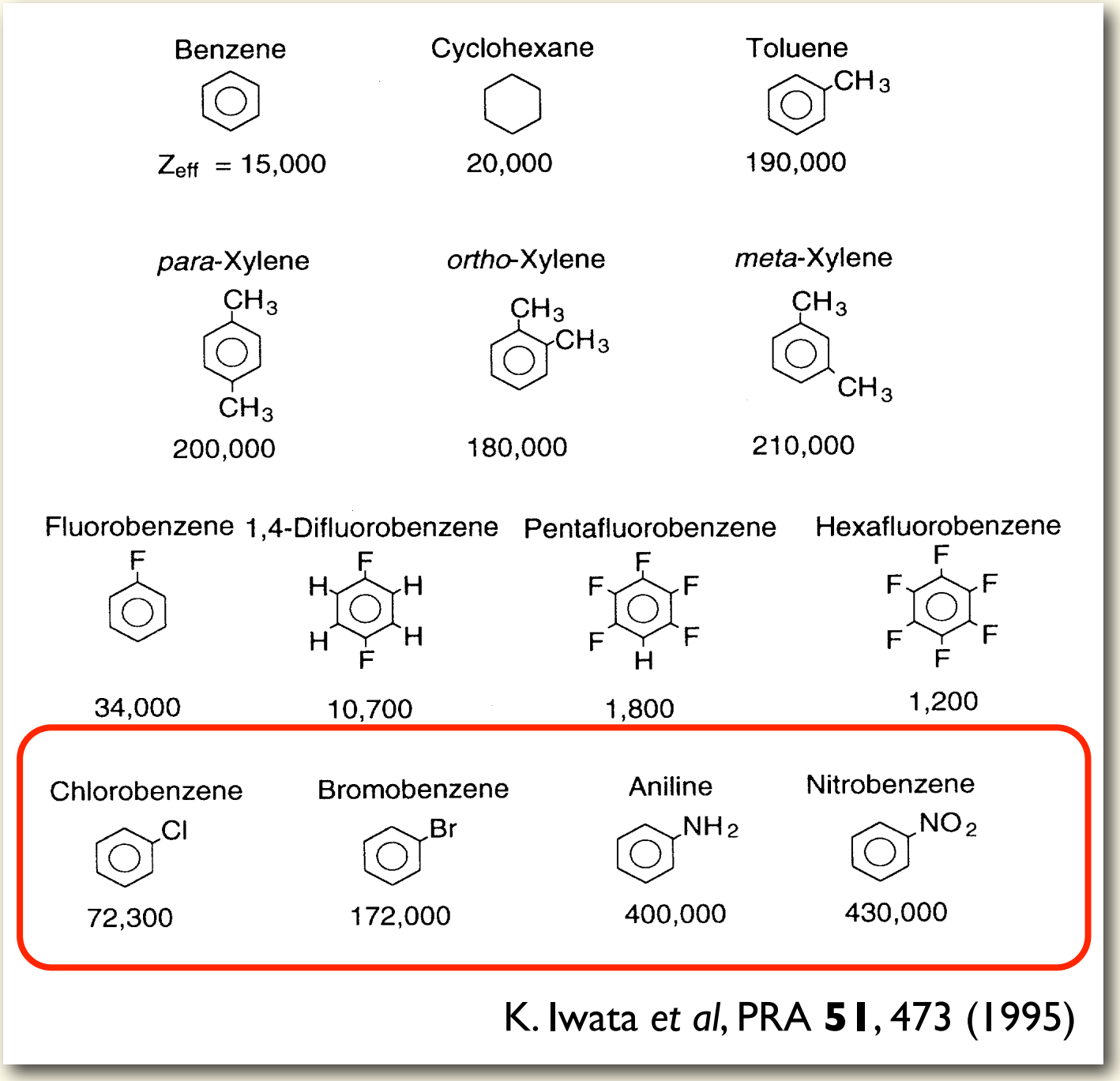

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Weakly bound positron states

$$\Psi_0(\mathbf{r}_1,\ldots,\mathbf{r}_Z,\mathbf{r}) \simeq \underbrace{\Phi_0(\mathbf{r}_1,\ldots,\mathbf{r}_Z)}_{\text{Atomic/molecular ground state}} \underbrace{A\frac{e^{-\kappa r}}{r}}_{\text{Positron wavefunction}}$$

$$\varepsilon_0 = -\frac{\kappa^2}{2}$$

Normalisation: $A \simeq \sqrt{\kappa/2\pi}$

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Annihilation rate

$$\Gamma^a = \pi r_0^2 c \rho_{ep}$$

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$F \sim 1$ in atomic units

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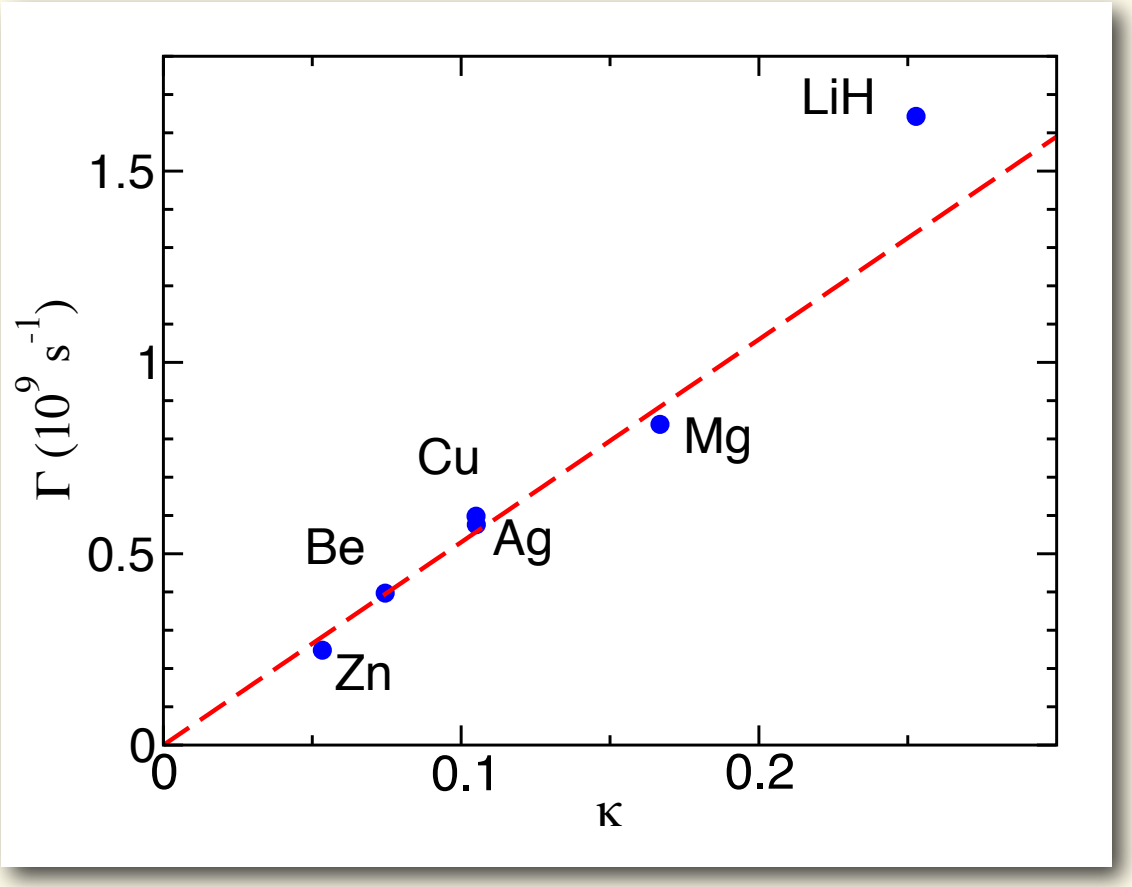

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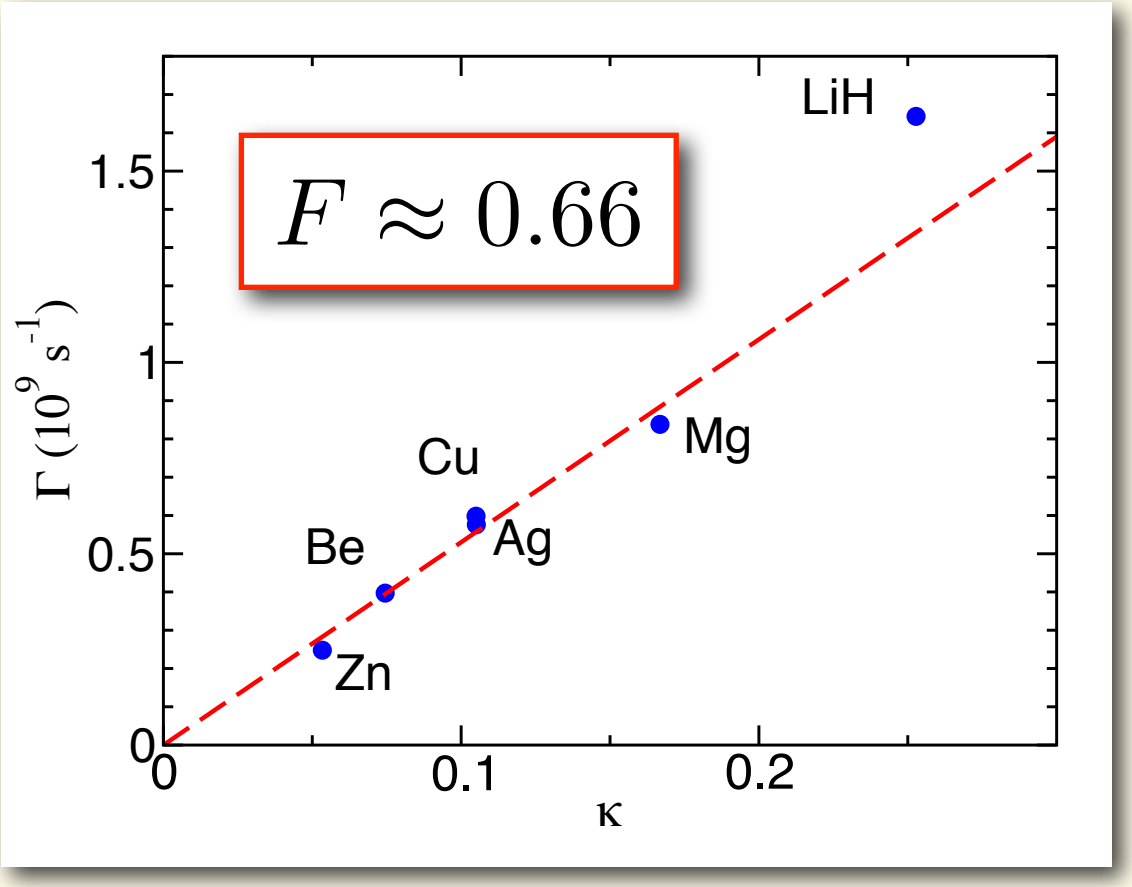
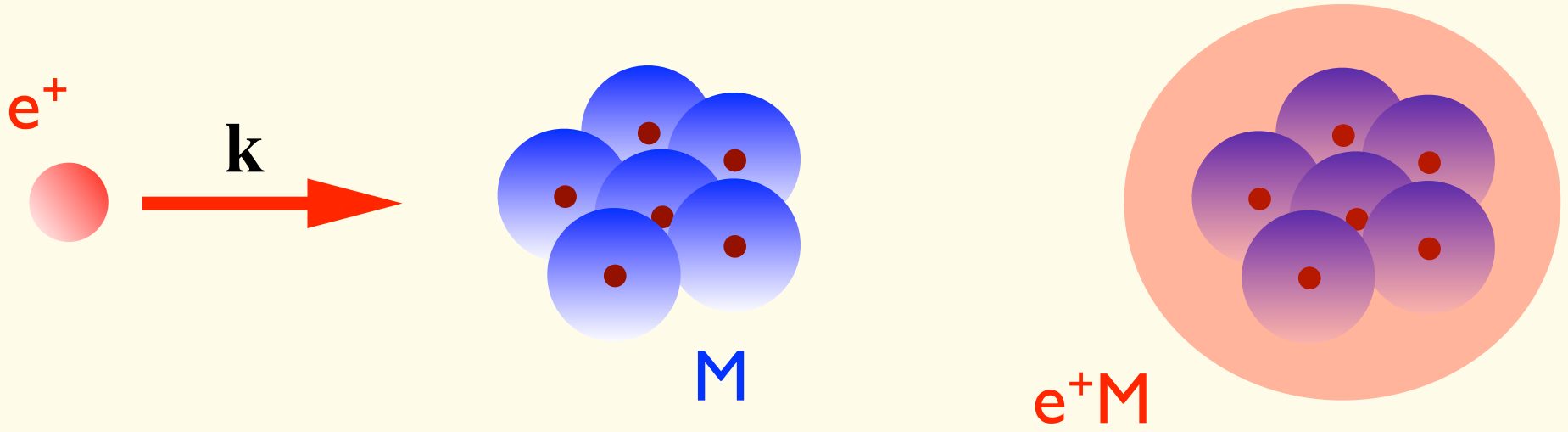


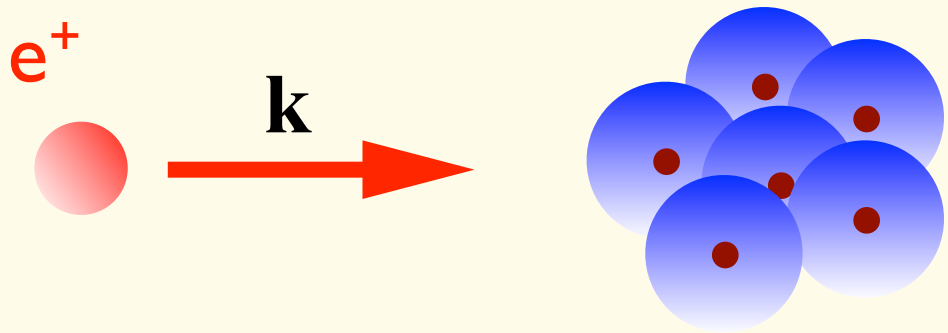
Resonant annihilation

Resonant annihilation

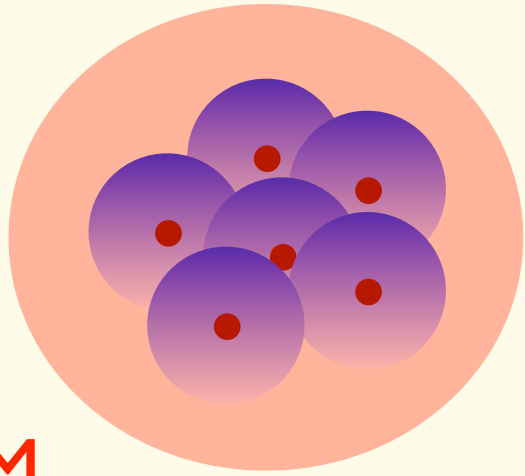


Vibrational Feshbach resonance

Resonant annihilation



M



e+M

Breit-Wigner theory

$$\sigma_a = \frac{\pi}{k^2} \sum_\nu \frac{g_\nu \Gamma_\nu^a \Gamma_\nu^e}{(\varepsilon - \varepsilon_\nu)^2 + \frac{1}{4}\Gamma_\nu^2}$$

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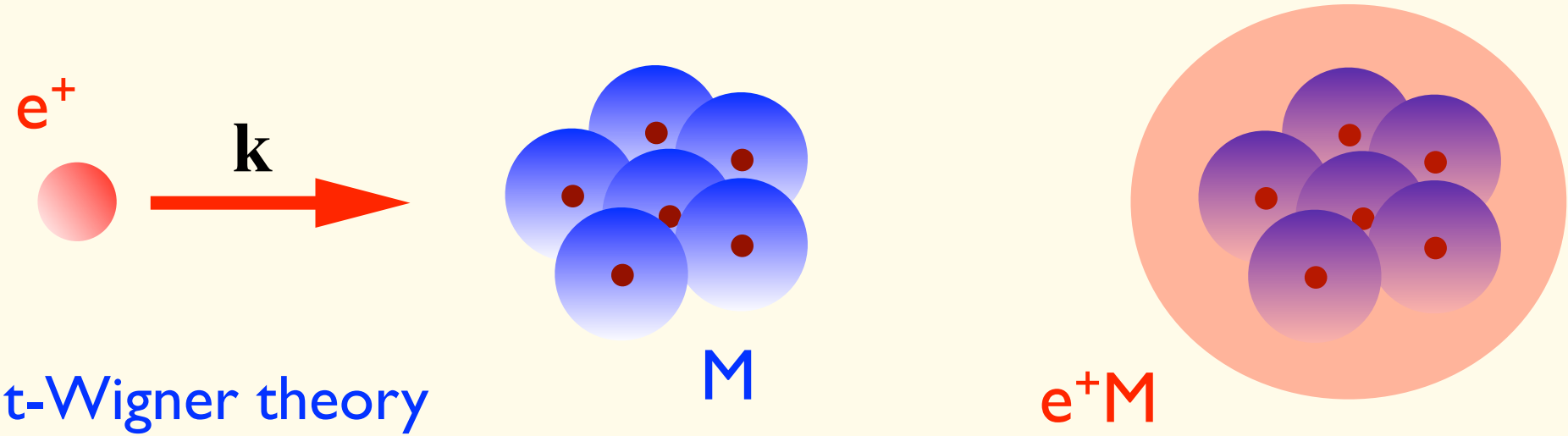

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$$e^+ + M(\nu_i) \longrightarrow Me^+(\nu) \xrightarrow{\Gamma_\nu^a} M^+ + 2\gamma$$

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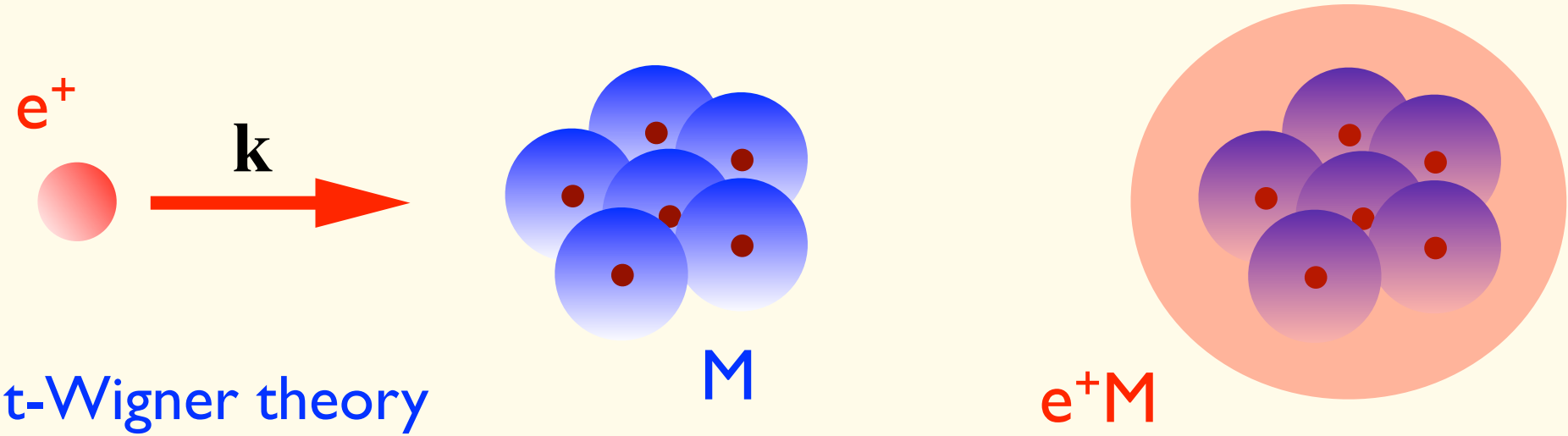

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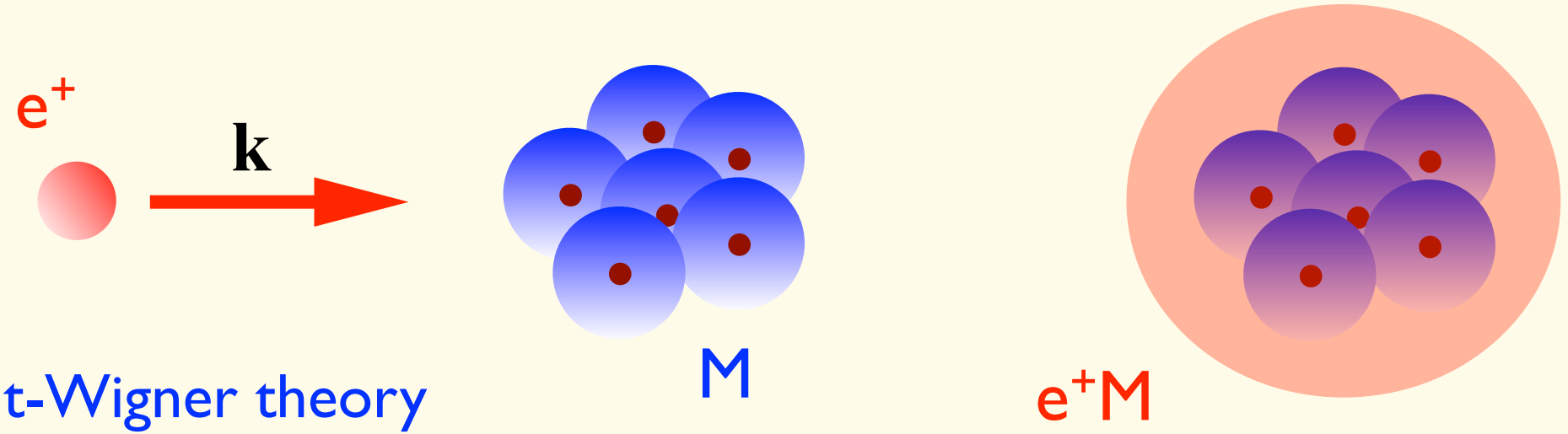

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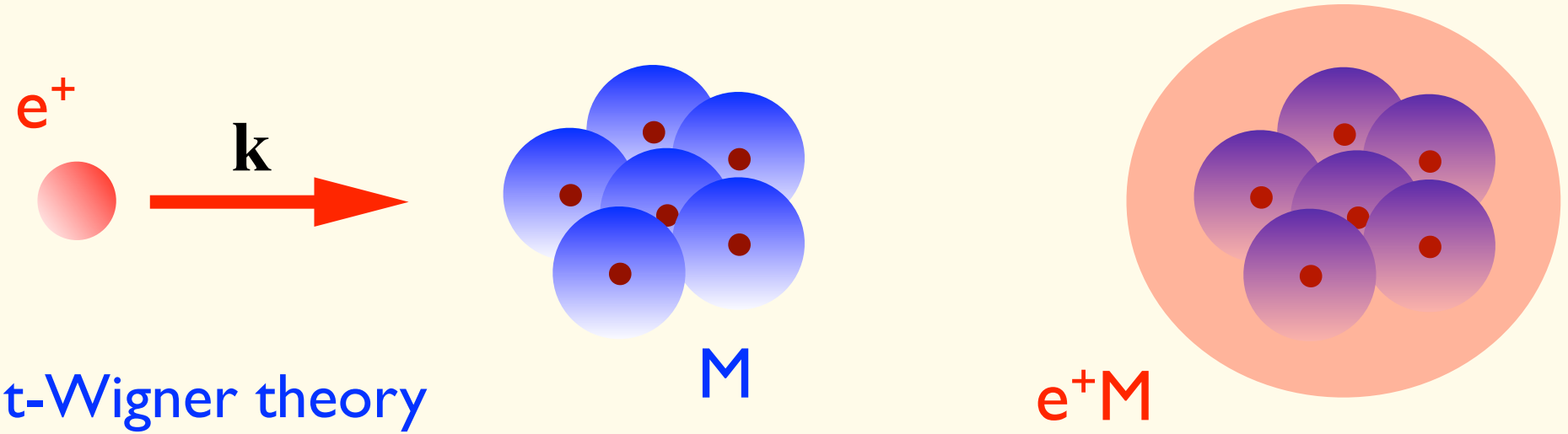

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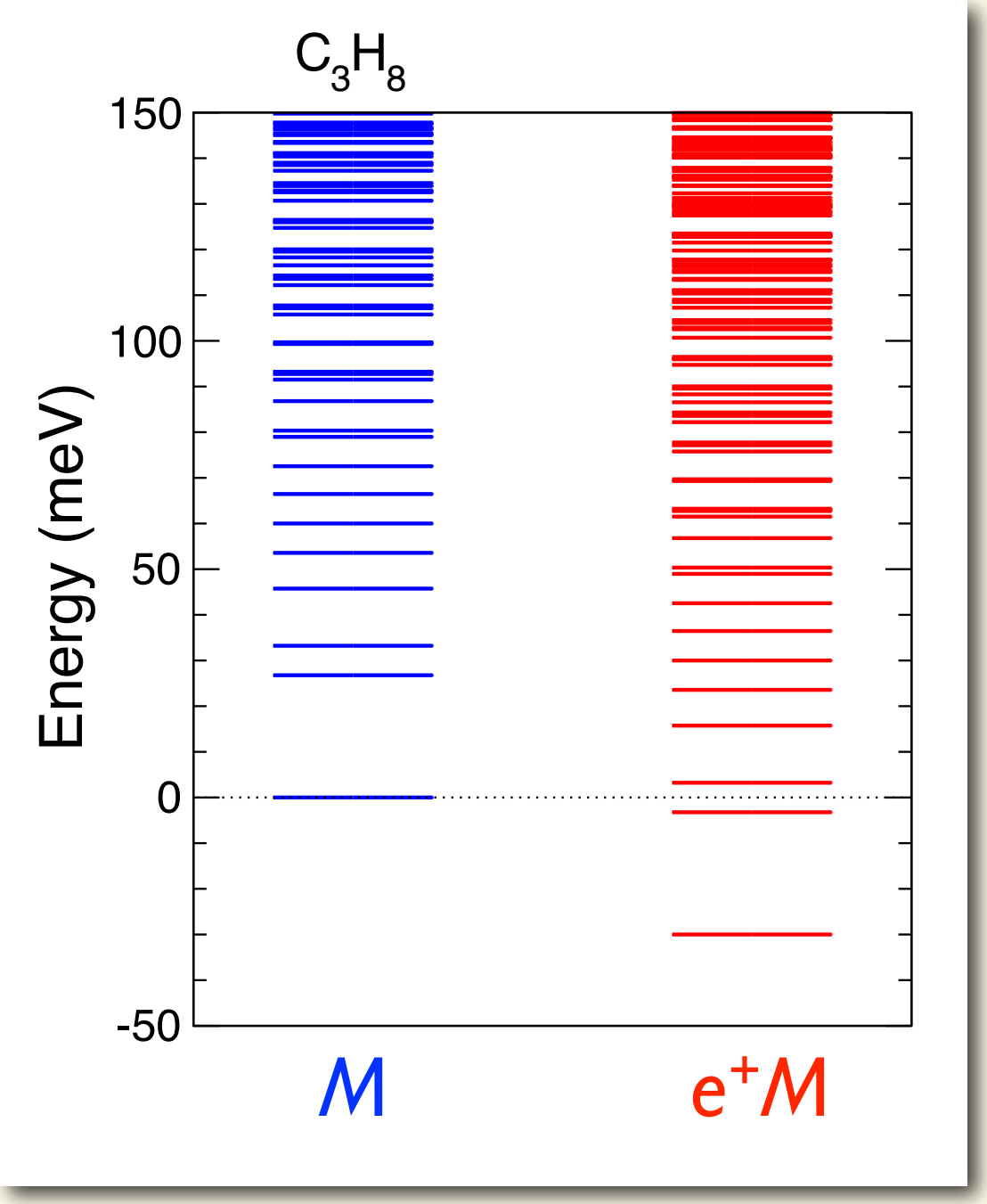
$$Me^+(\nu) \rightarrow M(\nu') + e^+$$

$$\varepsilon_\nu = E_\nu - E_{\nu_i} - \varepsilon_b$$

$$\Gamma_\nu = \Gamma_\nu^a + \Gamma_\nu^e + \sum_{\nu'} \Gamma_{\nu\nu'}^i$$

position and width of the resonances

Positron capture into dense spectrum of VFR



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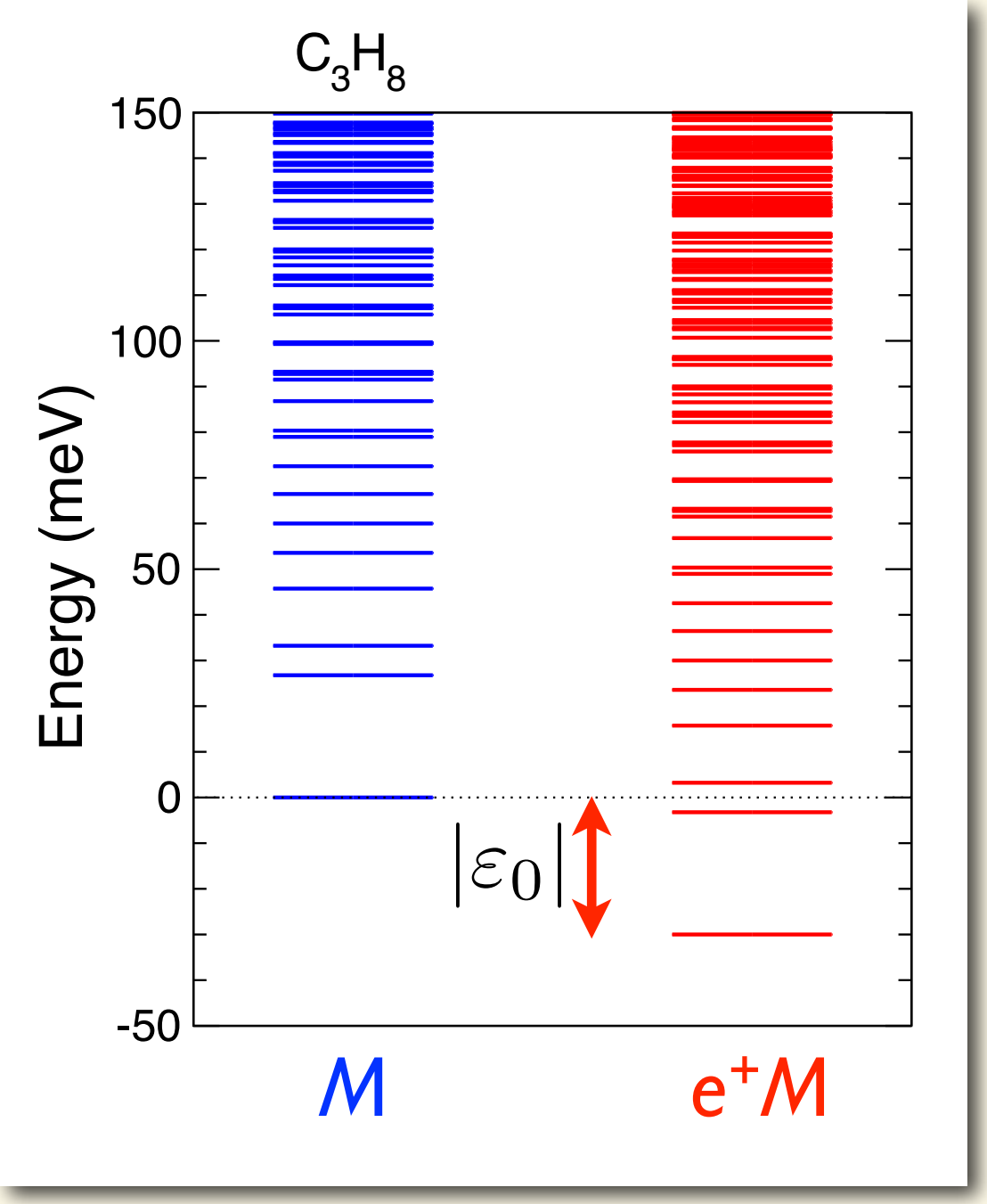

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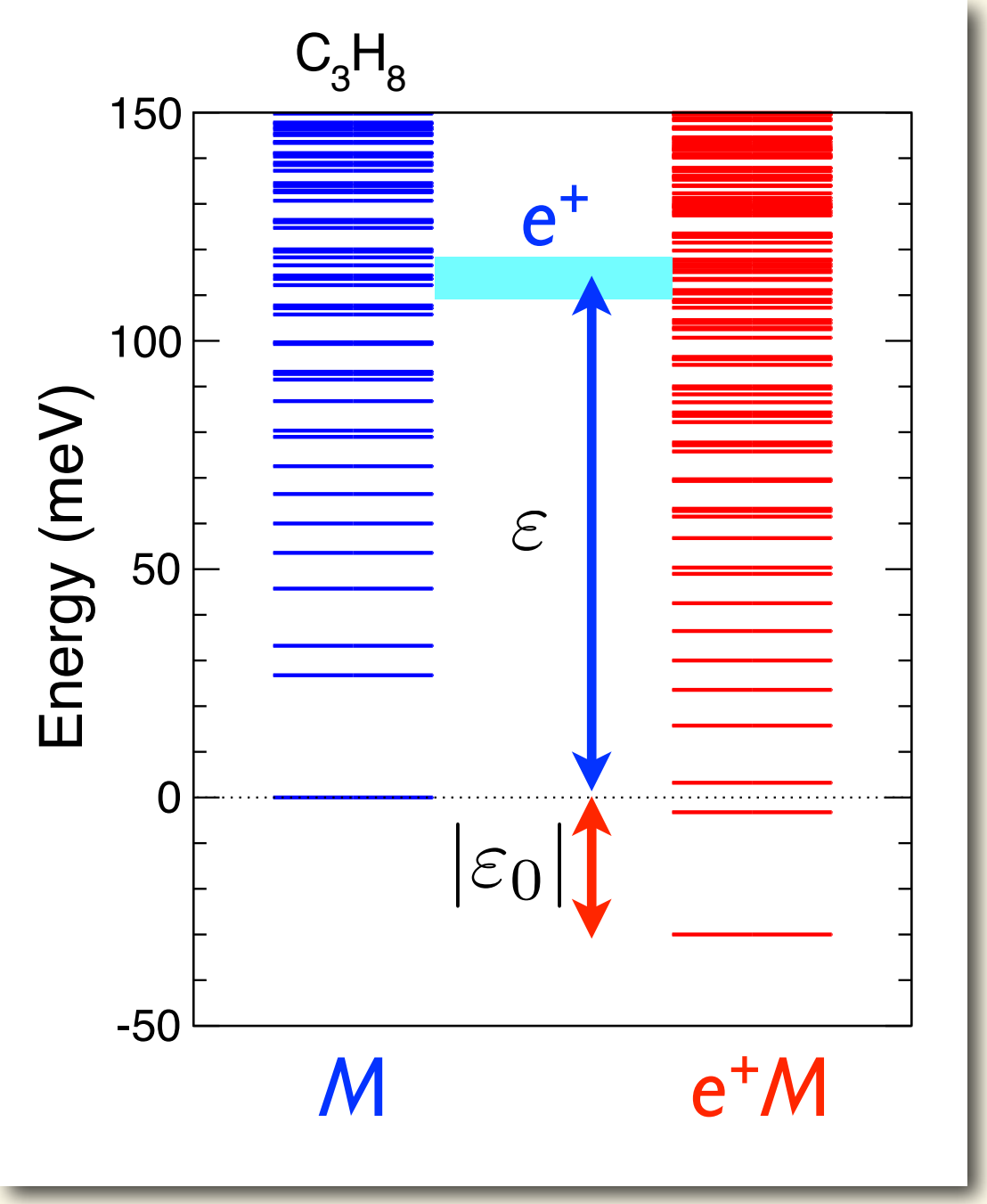

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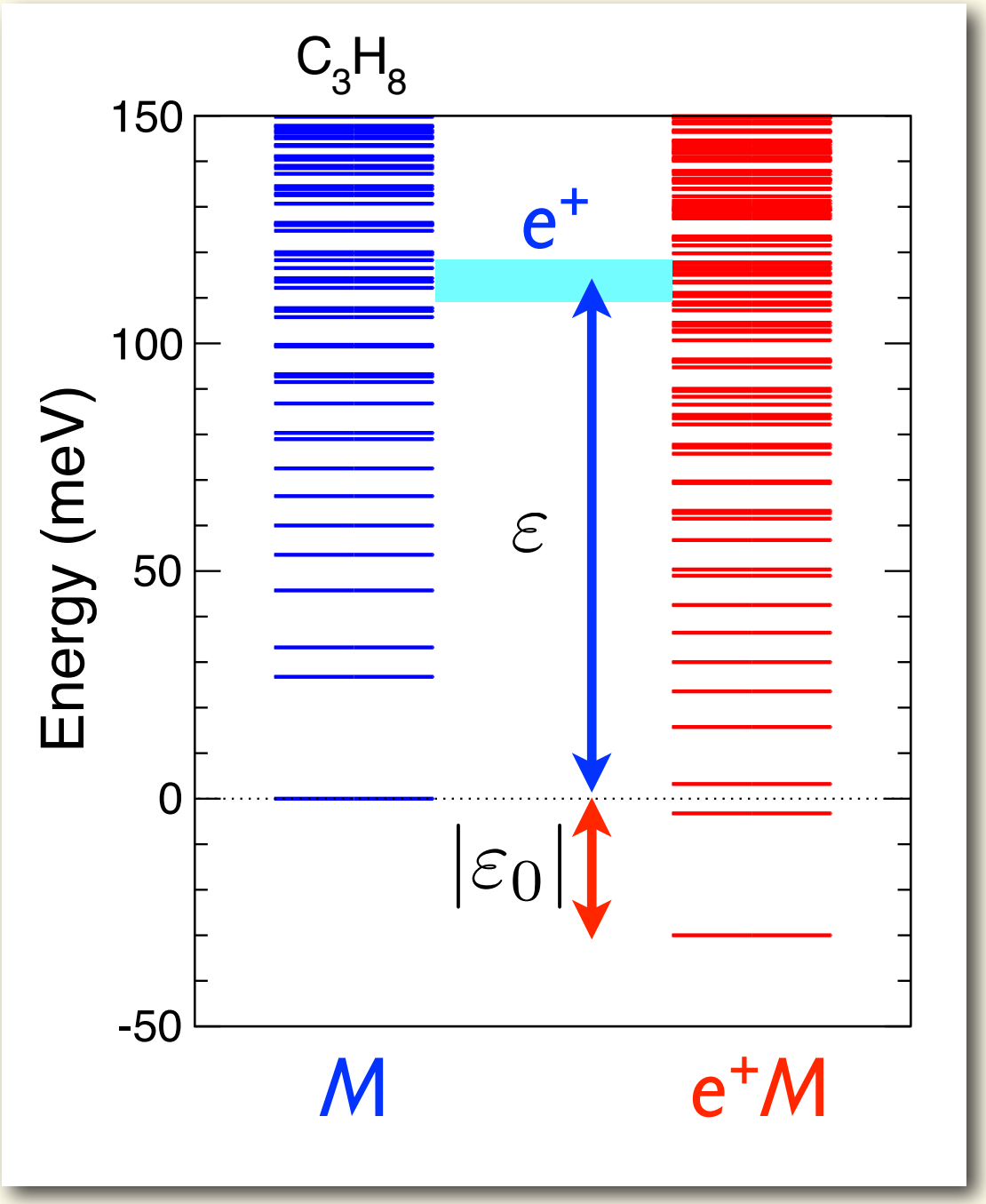

Averaging over positron energy spread

$$\bar{\sigma}_a = \frac{2\pi^2}{k^2}\frac{\Gamma^a\Gamma^e(\varepsilon)}{\Gamma(\varepsilon)}\rho(E)$$

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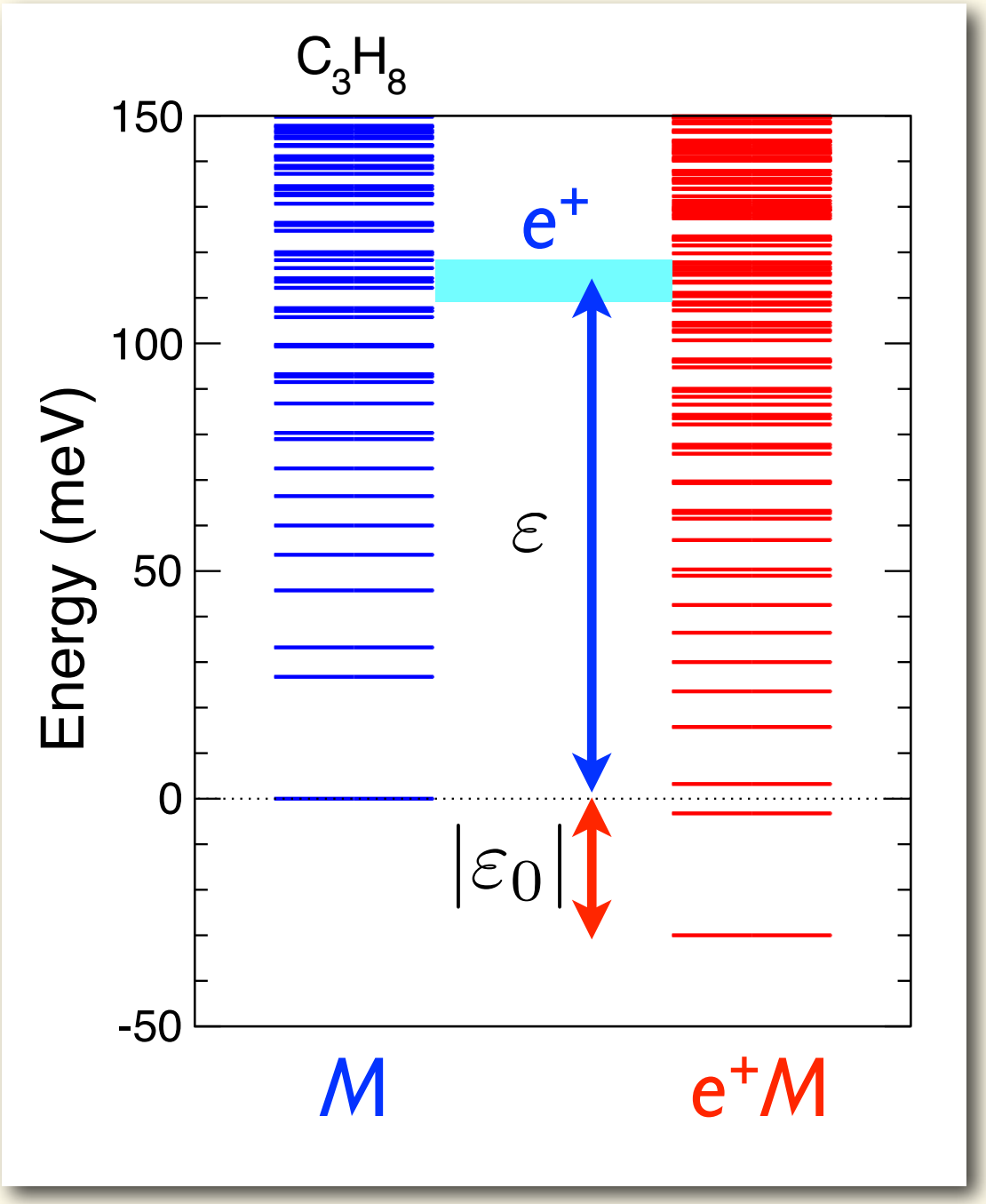

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vibrational spectrum density of e^+M at

$$E = \varepsilon + |\varepsilon_0| + E_{\nu_i}$$

Resonant annihilation in alkanes

$$Z_{\text{eff}} = \frac{2\pi^2 \rho_{ep}}{k} \frac{\Gamma^e(\varepsilon)}{\Gamma(\varepsilon)} \rho(E)$$

$$Z_{\text{eff}} = \pi F \sqrt{\frac{|\varepsilon_0|}{\varepsilon}} \frac{\rho(\varepsilon + |\varepsilon_0| + E_{\nu_i})}{N(\varepsilon + E_{\nu_i})}$$

$$N(E) = \int_0^E \rho(E')dE'$$

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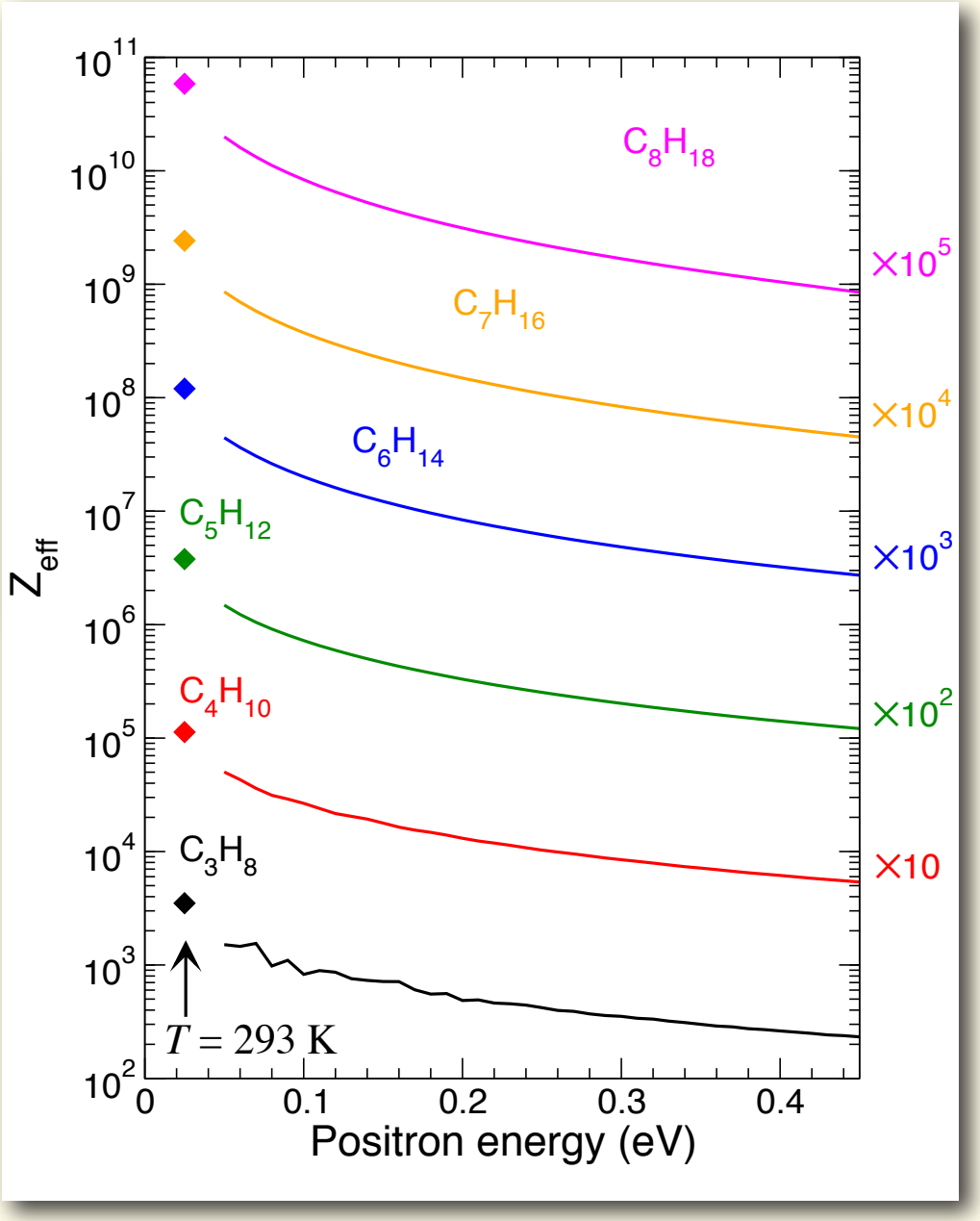

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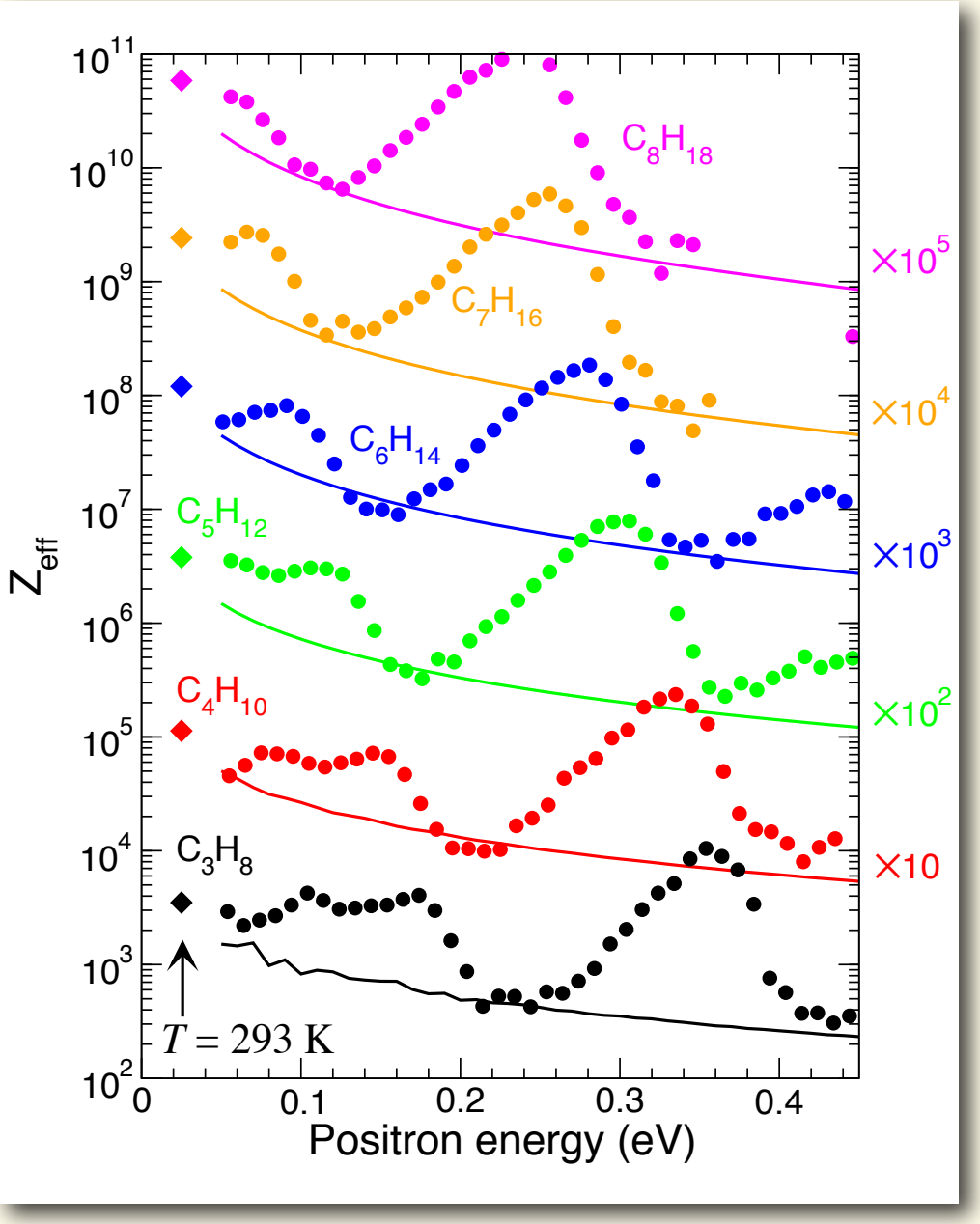
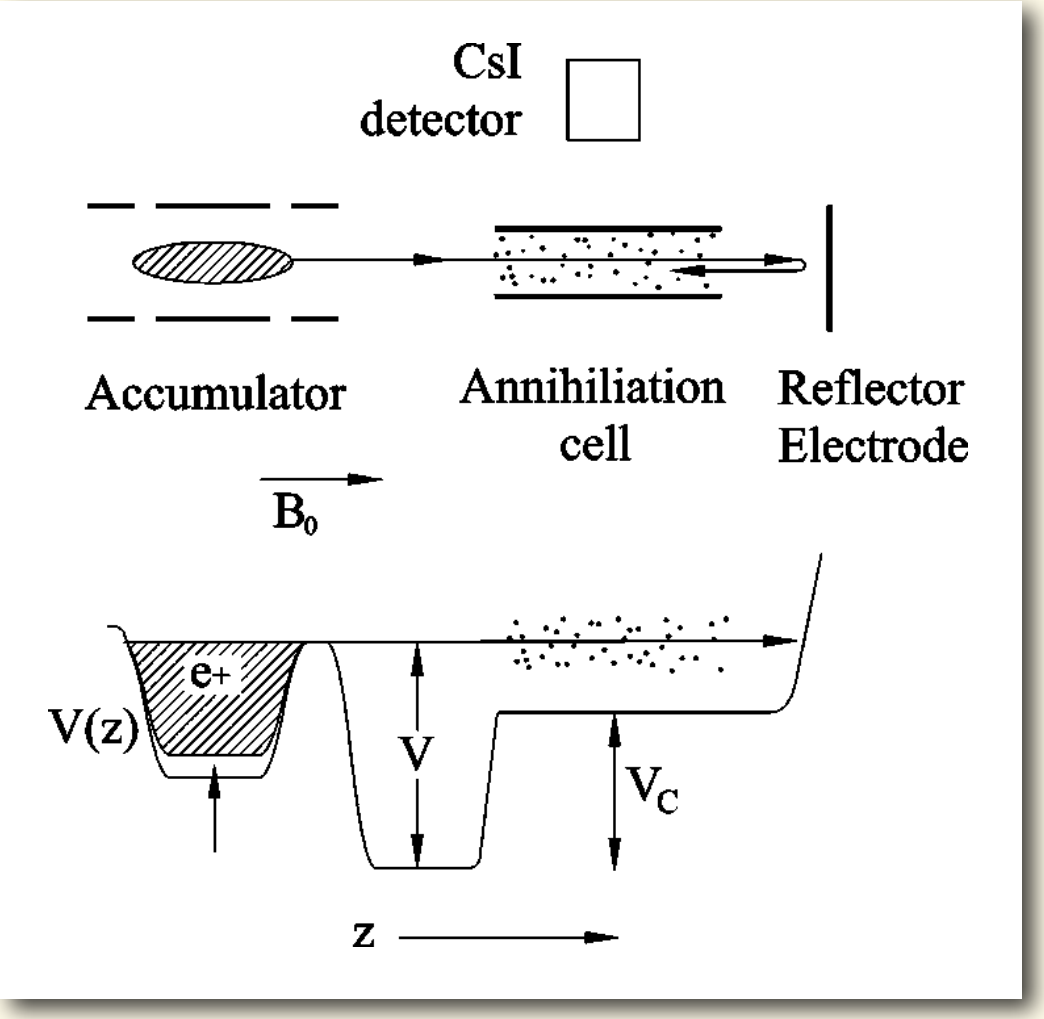


Measuring Z_{eff} as a function of positron energy

S. J. Gilbert, L. D. Barnes, J. P. Sullivan and C. M. Surko, Phys. Rev. Lett. **88**, 043201 (2002)



By reducing the depth of the trap, the positrons are "pushed" over the edge to form a beam

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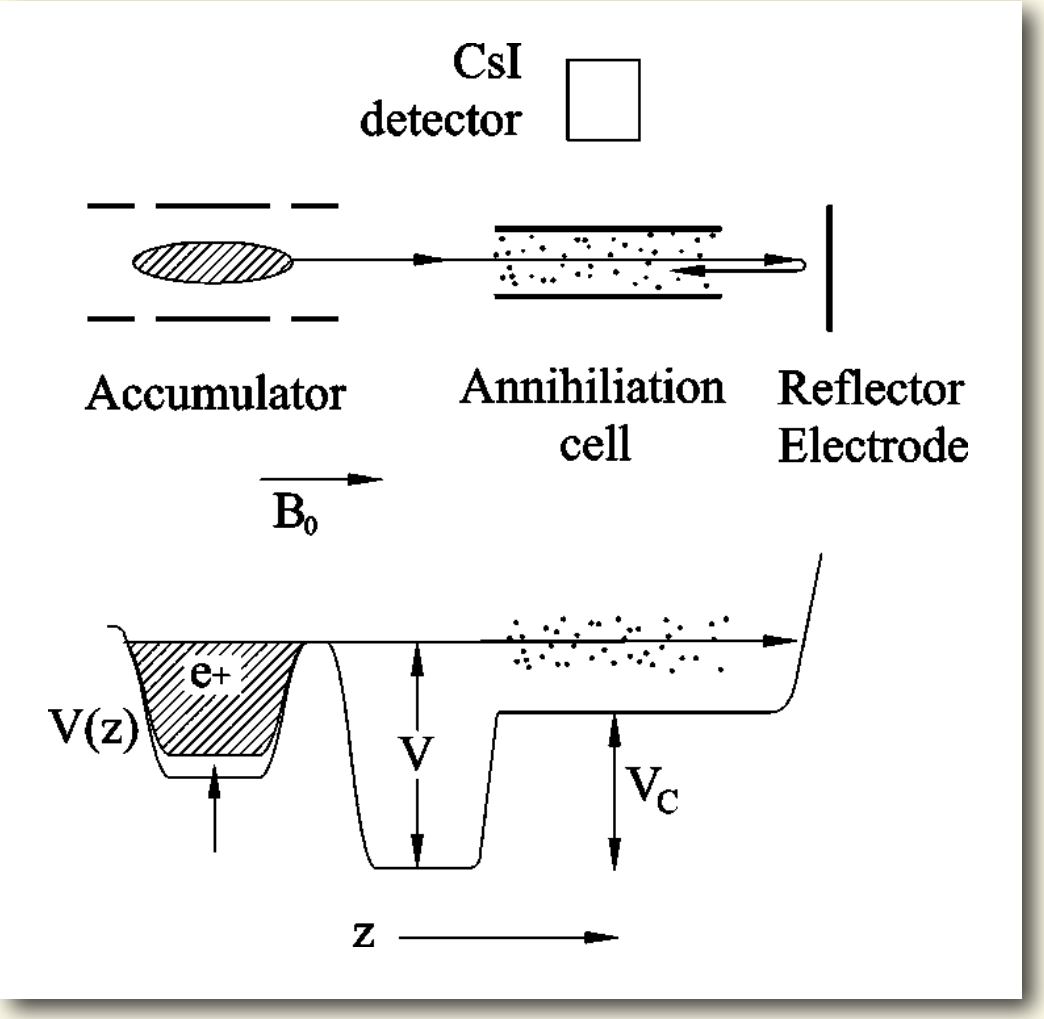

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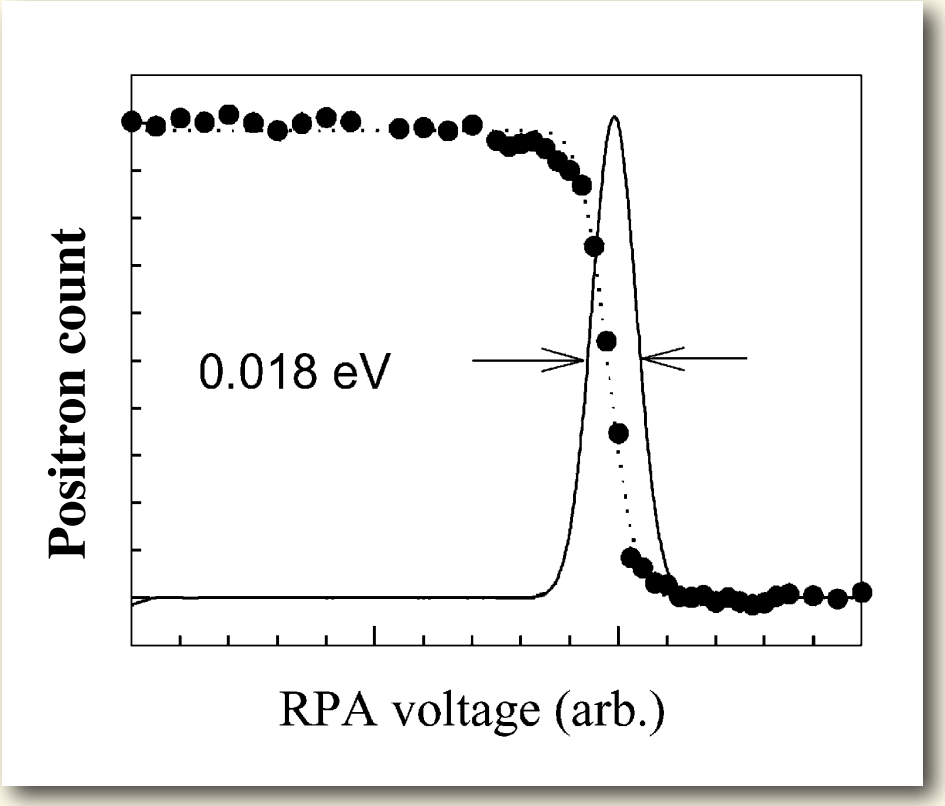
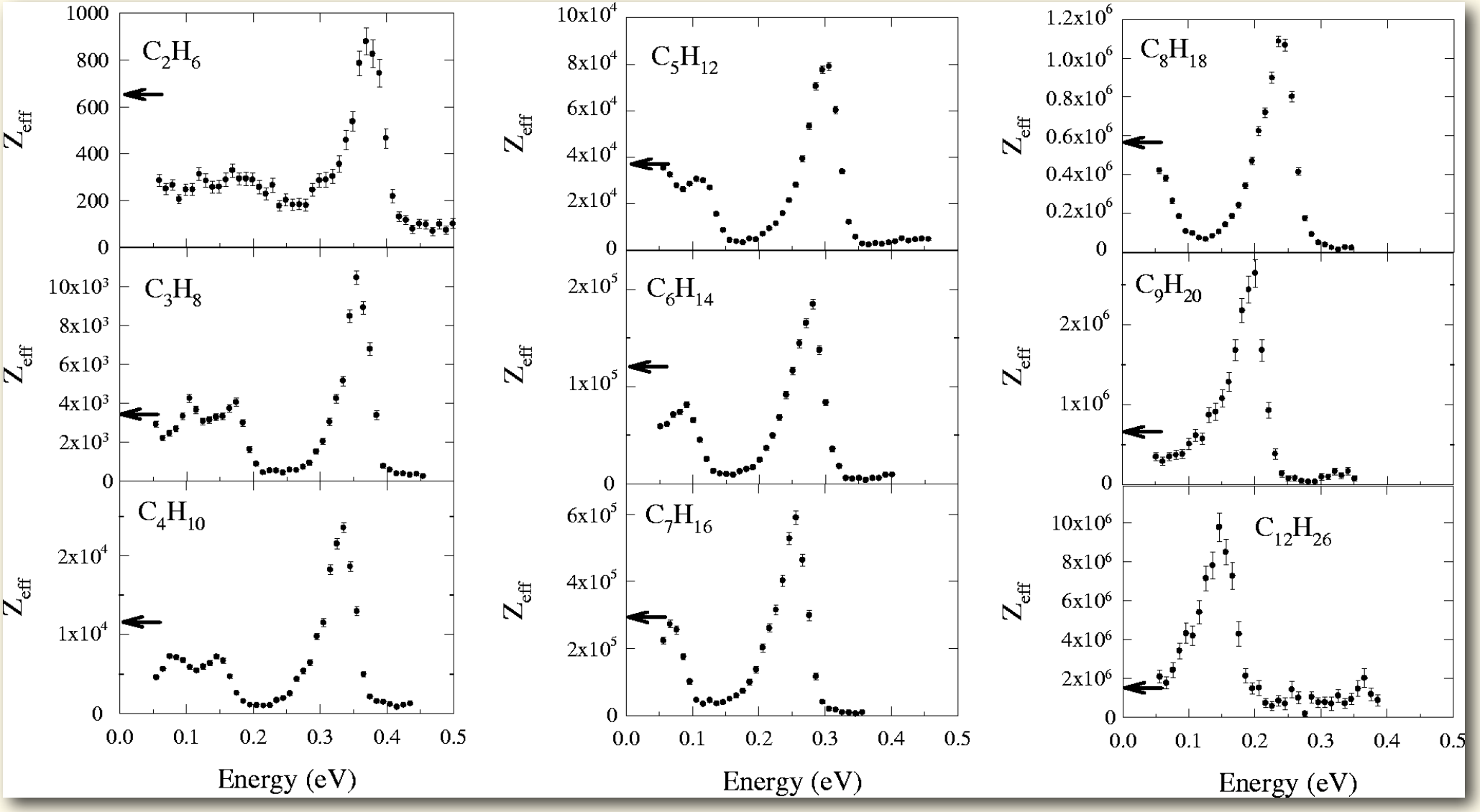


Positron parallel energy distribution is approximately Gaussian with FWHM ~ 25 meV

S. J. Gilbert et al., Appl. Phys. Lett. **70**, 1944 (1997)

Dependence of Z_{eff} on positron energy for alkanes



Barnes et al. PRA **67**, 032706 (2003)

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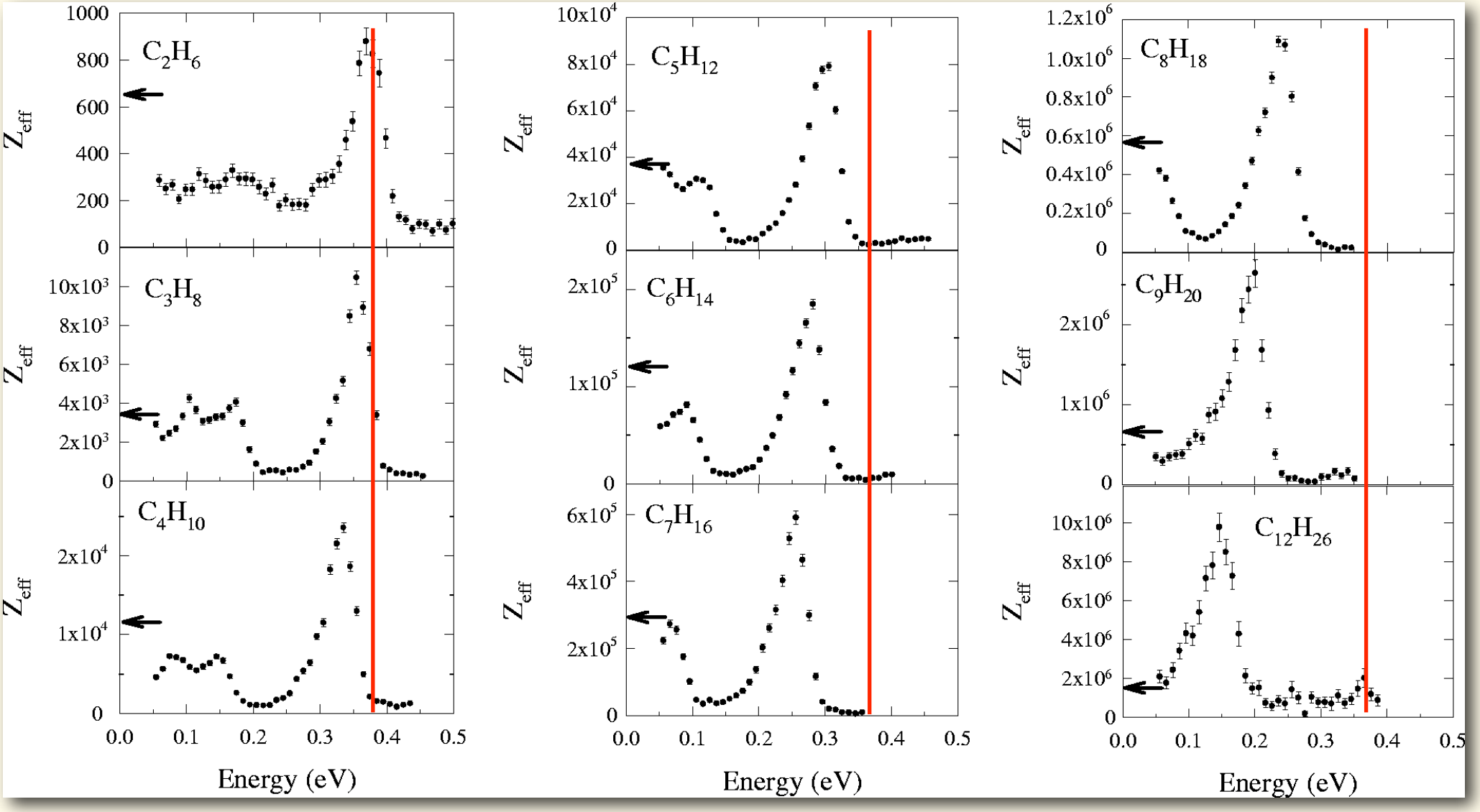
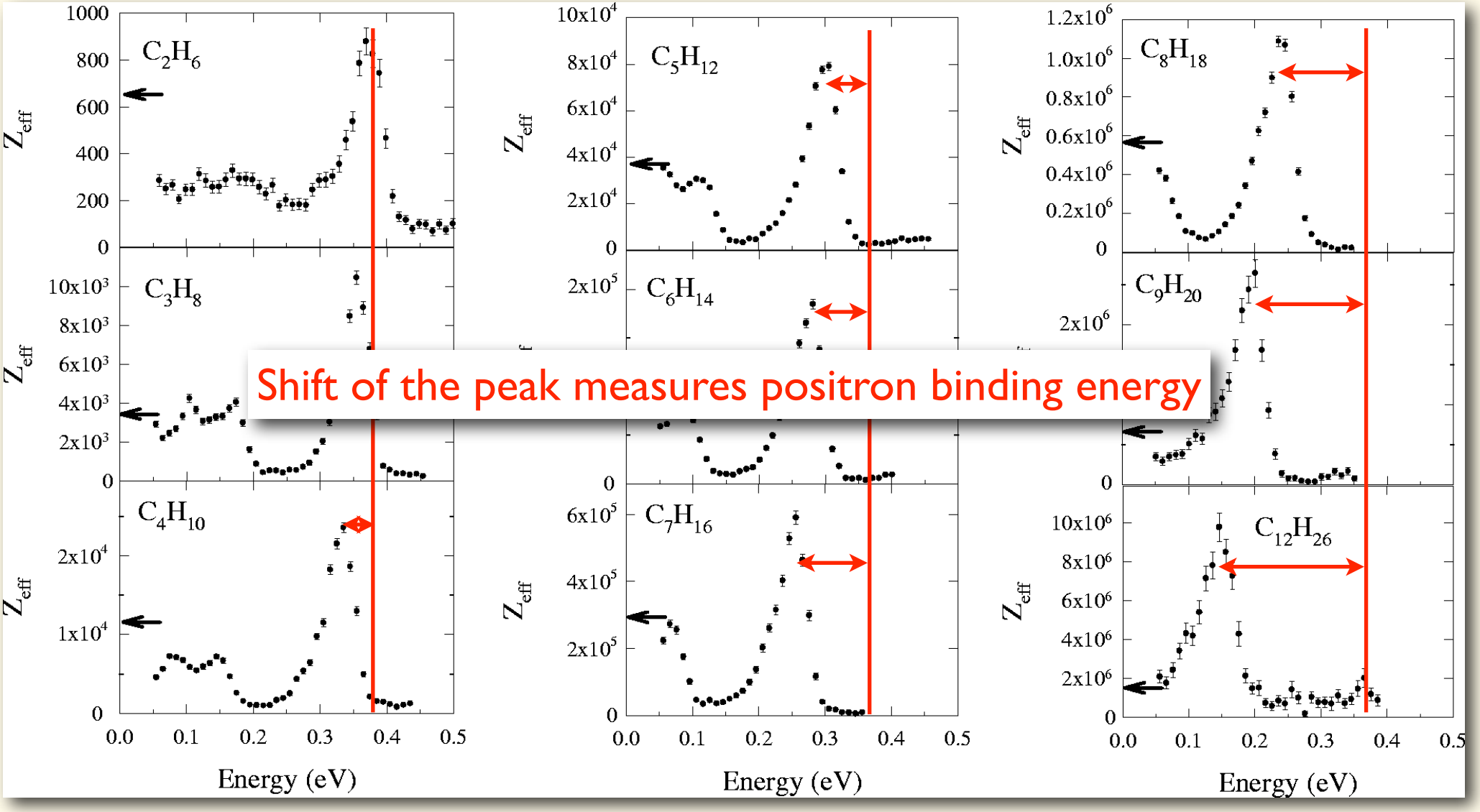


C-H vibrational mode $\omega \approx 0.37$ eV

Barnes et al. PRA **67**, 032706 (2003)

Dependence of Z_{eff} on positron energy for alkanes



C-H vibrational mode $\omega \approx 0.37$ eV

Barnes et al. PRA **67**, 032706 (2003)

Positron capture by VFR of infrared-active modes

G. F. Gribakin and C. M. R. Lee, Phys. Rev. Lett. **97**, 193201 (2006)

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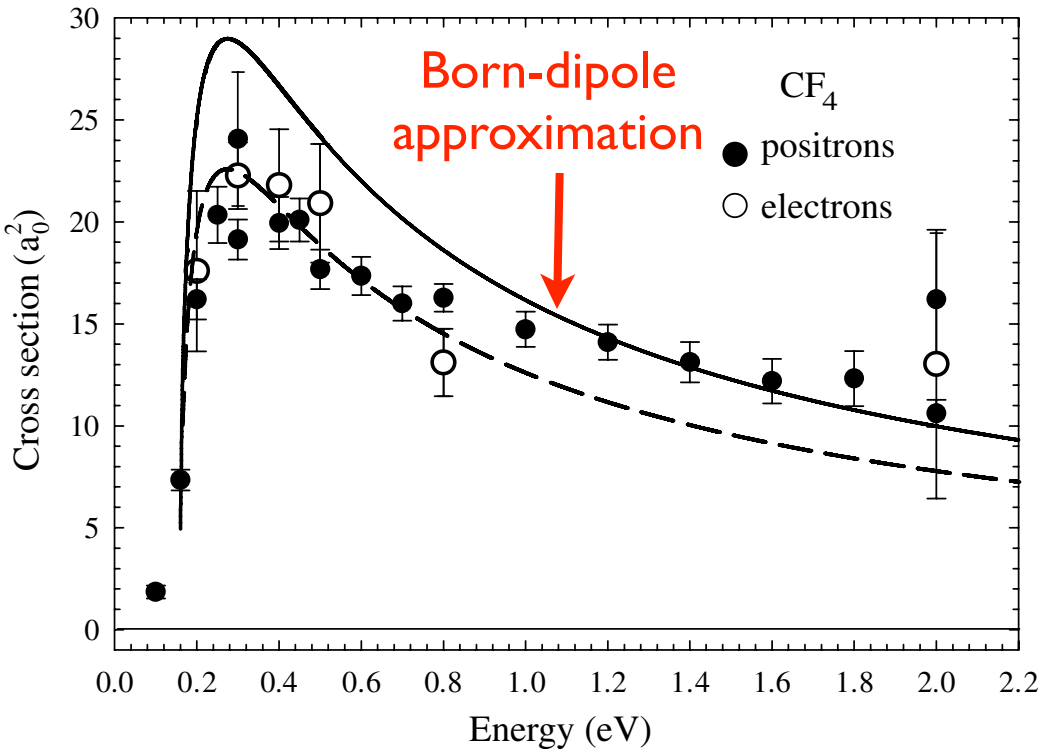

Marler, Gribakin and Surko, NIMB **247**, 87 (2006)

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$$\Gamma^e_\nu = 2\pi \int |A_{\nu\mathbf{k}}|^2 \delta(k^2/2 - \omega_\nu - \varepsilon_0)\frac{d^3k}{(2\pi)^3}$$

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Fundamentals and elastic widths in CH_3Cl

TABLE I. Characteristics of the vibrational modes of CH_3Cl.

Mode	Symmetry	g_ν	ω_ν [a] (meV)	d_ν (a.u.)	$\omega_\nu d_\nu^2$ (a.u.)
ν_1	a_1	1	363	0.0191	4.87×10^{-6}
ν_2	a_1	1	168	0.0176	1.91×10^{-6}
ν_3	a_1	1	91	0.0442	6.52×10^{-6}
ν_4	e	2	373	0.0099	1.34×10^{-6}
ν_5	e	2	180	0.0162	1.74×10^{-6}
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[a]Mode energies ω_ν and dipole amplitudes d_ν from Ref. [29].

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Annihilation width vs elastic width: $|\varepsilon_0| = 25$ meV

$\kappa = 0.043$ a.u. $\Gamma^{(a)} = 5.5 \times 10^{-9}$ a.u. $\ll \Gamma^{(e)}$

Putting it all together: total $Z_{\rm eff}$

$$Z_{\rm eff} = \bar{Z}^{\rm (res)}_{\rm eff} + \bar{Z}^{\rm (dir)}_{\rm eff}$$

$$Z^{\rm (res)}_{\rm eff} = \frac{\pi}{k}\rho_{ep}\sum_{\nu}\frac{g_\nu \Gamma^e_\nu}{(\varepsilon - E_\nu - \varepsilon_0)^2 + \Gamma^2_\nu/4} \qquad Z^{\rm (dir)}_{\rm eff} = \frac{F}{\kappa^2 + k^2}$$

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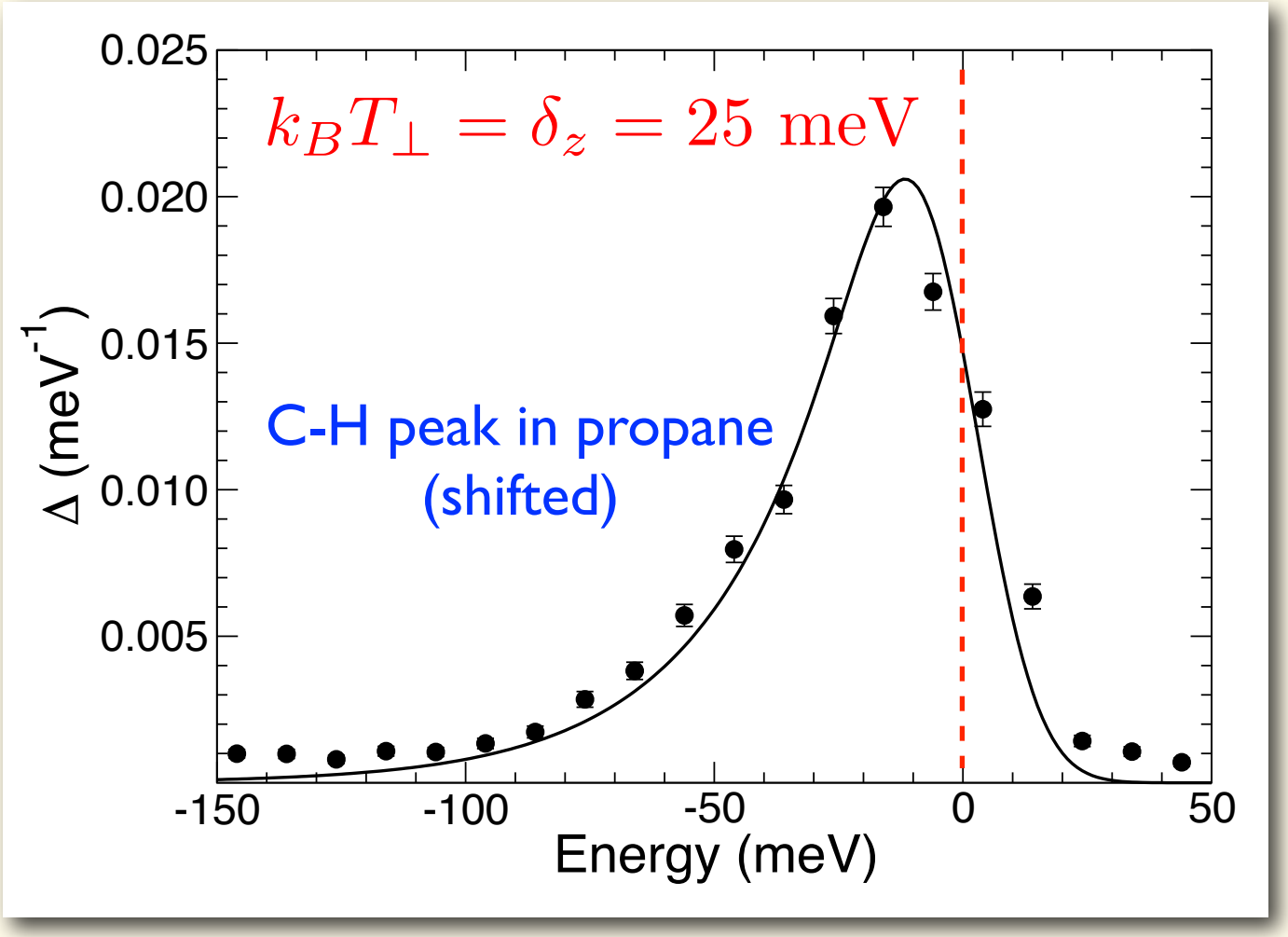
Function $\Delta\,(E)$ describes the shape of a resonance as observed with the beam

$$\Delta(E) = \frac{1}{2k_B T_\perp} \exp\left[\frac{\sigma^2}{2(k_B T_\perp)^2} + \frac{E}{k_B T_\perp}\right]\left\{1 + \Phi\left[-\frac{1}{\sqrt{2}}\left(\frac{E}{\sigma} + \frac{\sigma}{k_B T_\perp}\right)\right]\right\}$$

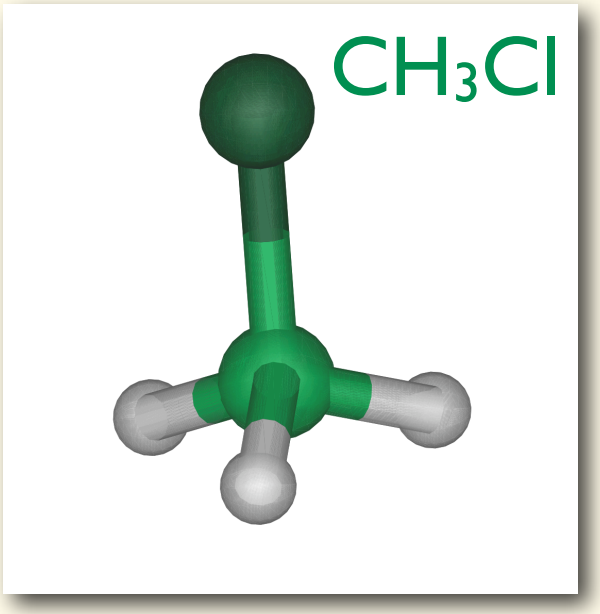
Shapes of resonances observed with cold positron beam



Theory vs experiment for halomethanes

Halogen-substituted methane: CH_3Hal

all 6 vibrational modes infrared active



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[Barnes, Gilbert and Surko, PRA **67** 032706 (2003)]

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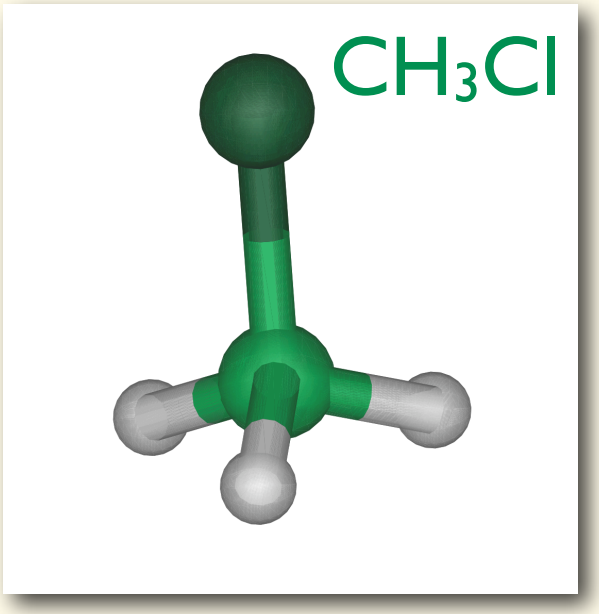

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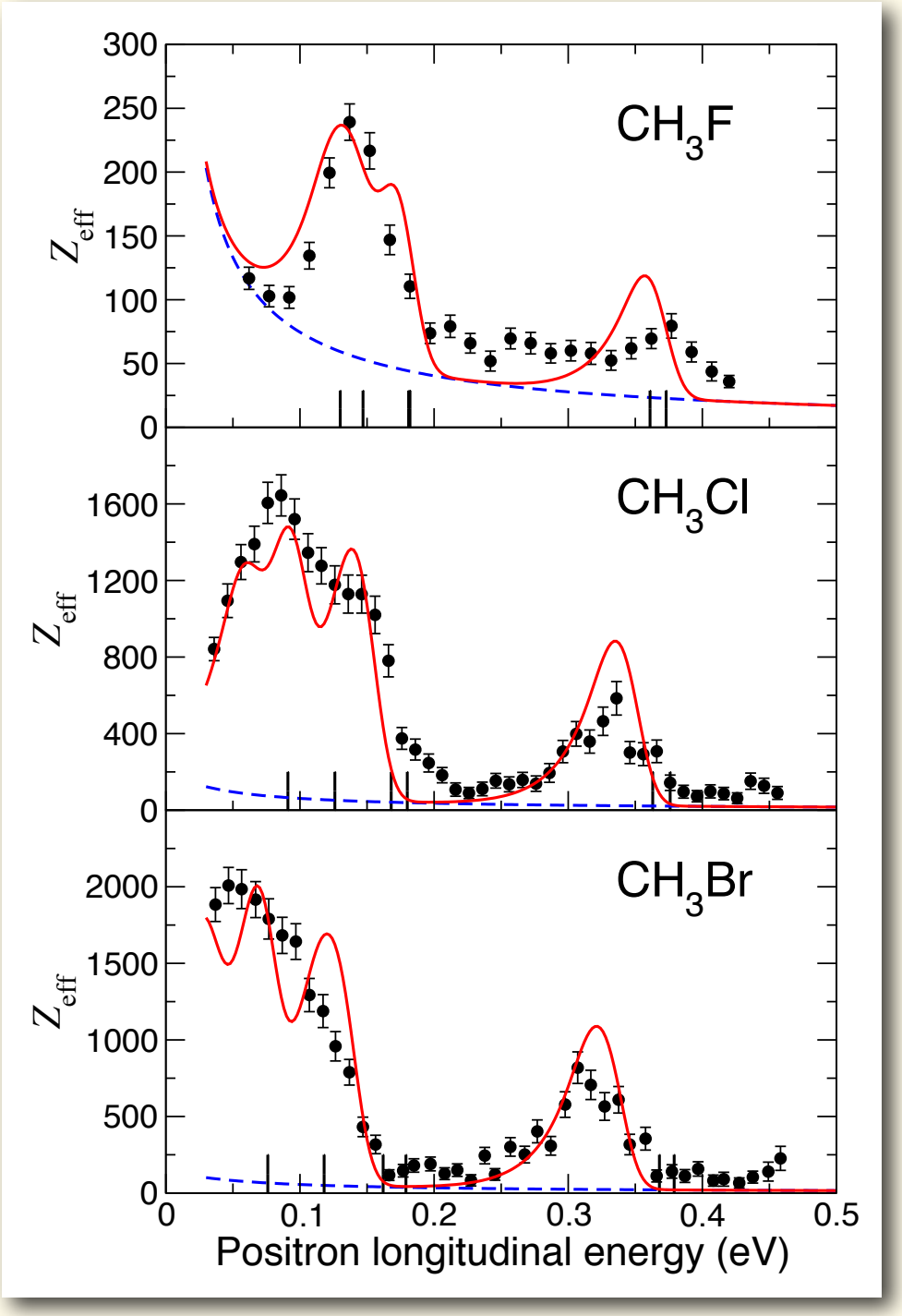

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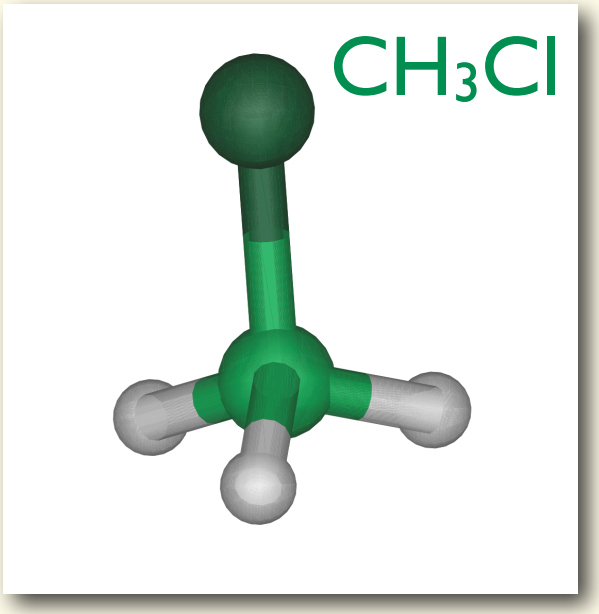

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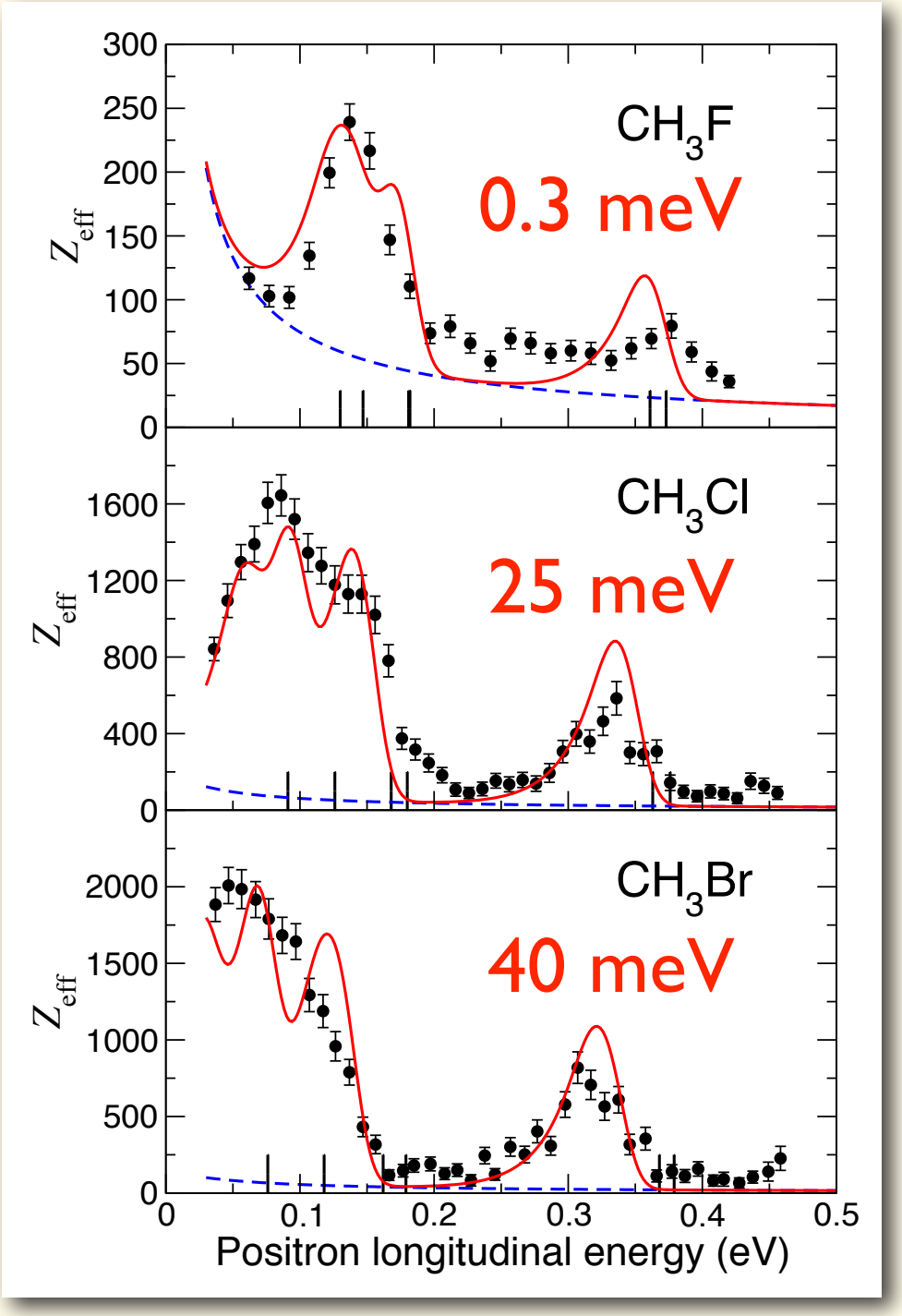
Binding energies are determined!



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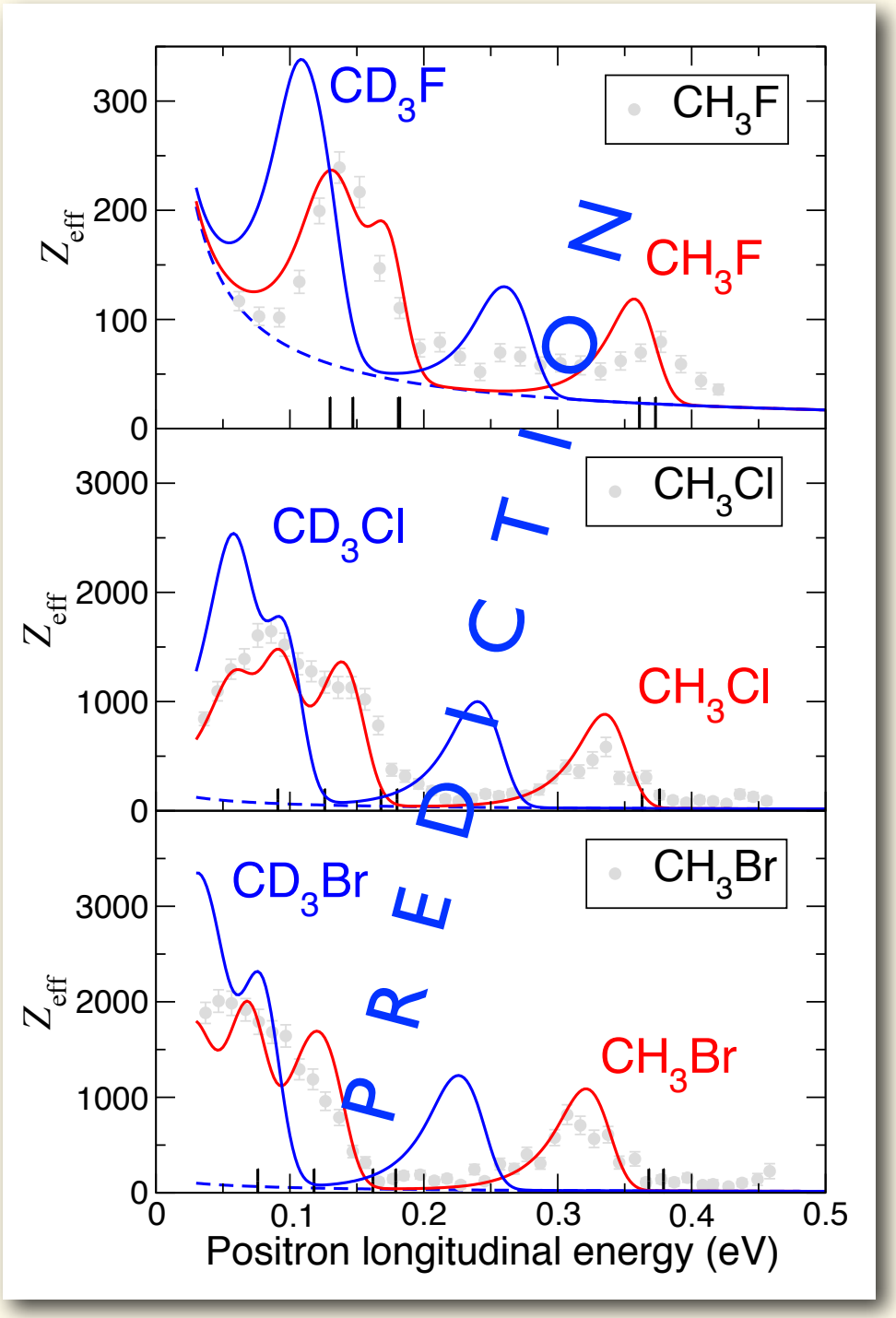

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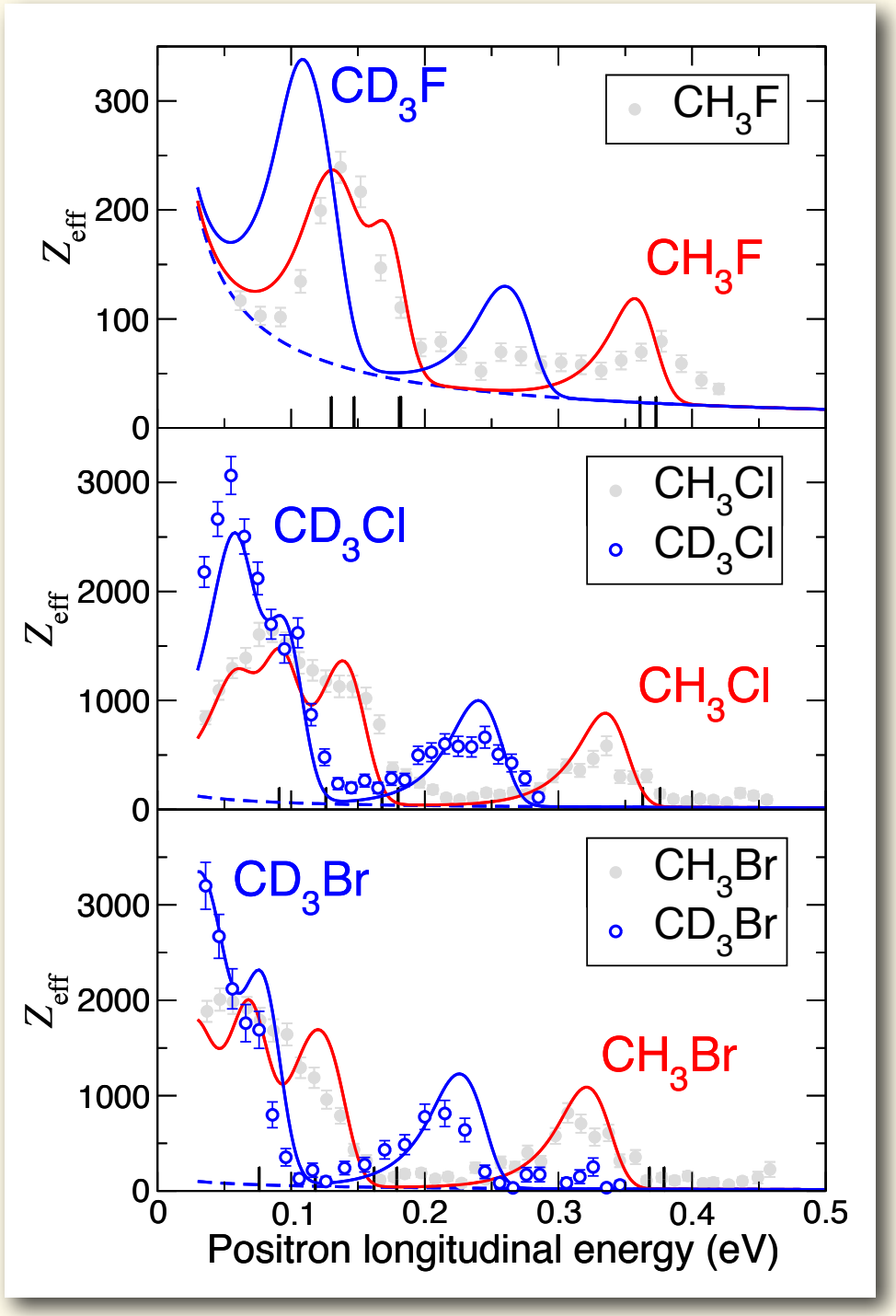

Young, Gribakin, Lee and Surko, Phys. Rev. A **77**, 060702 (2008)

Some other molecules

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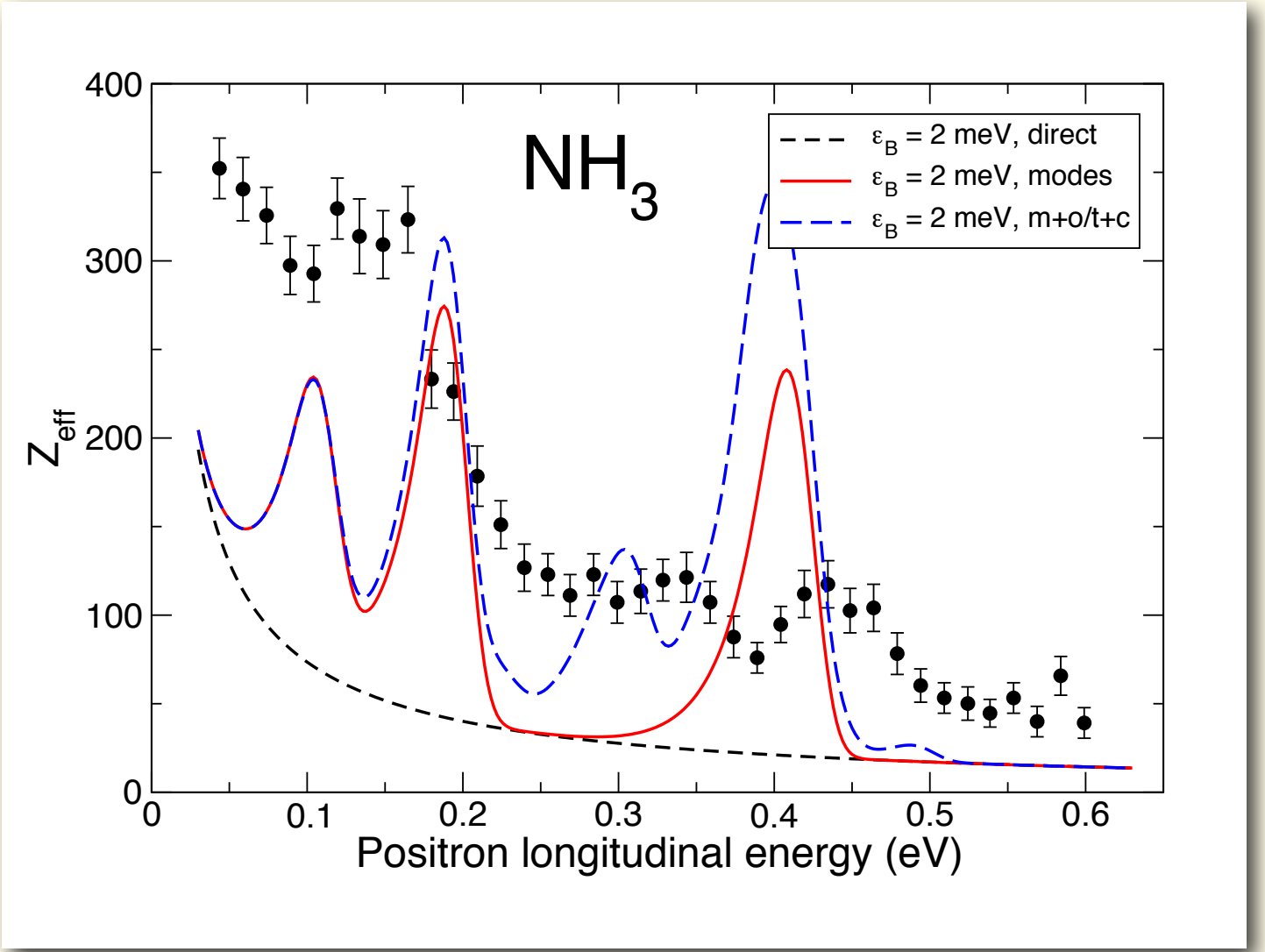

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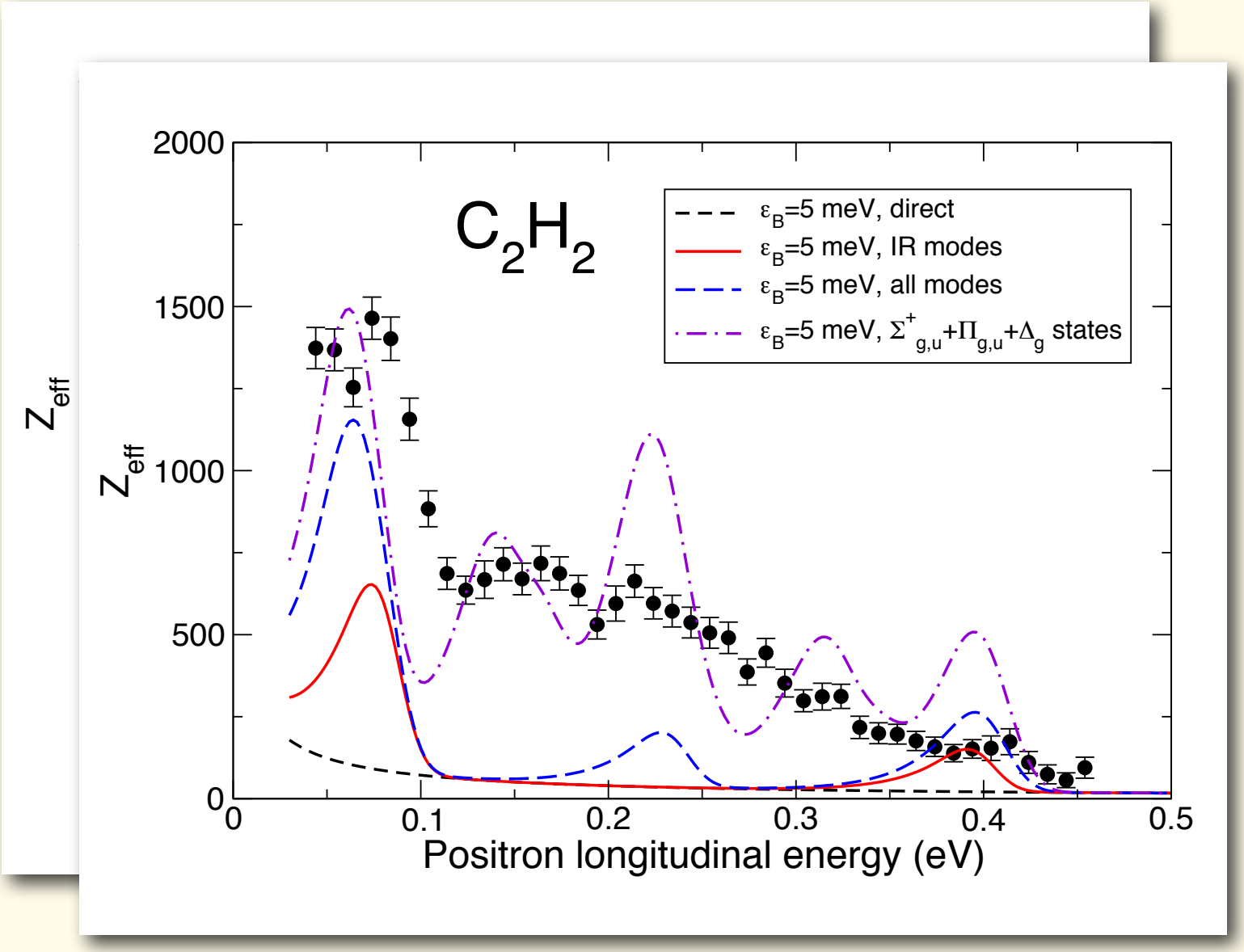

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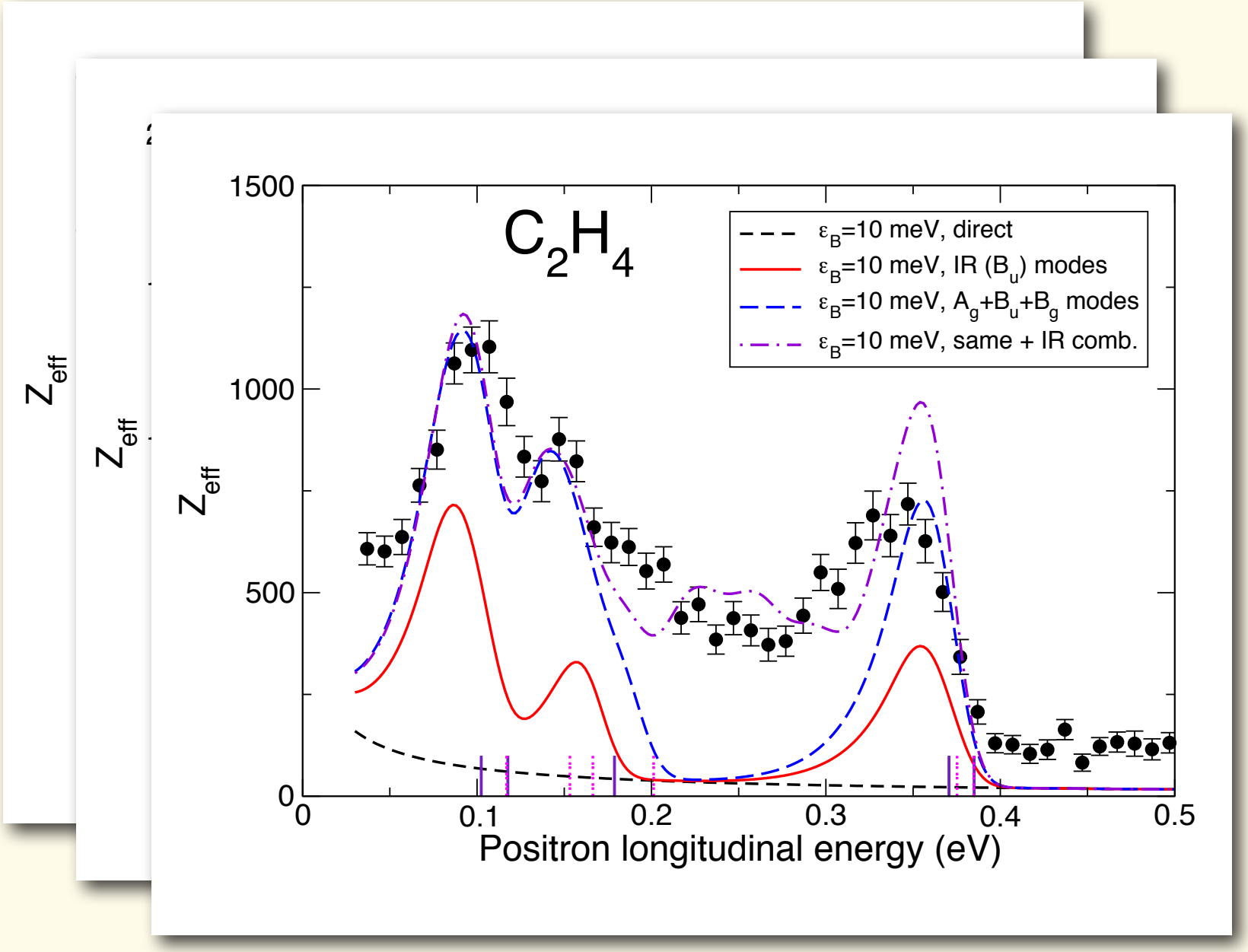

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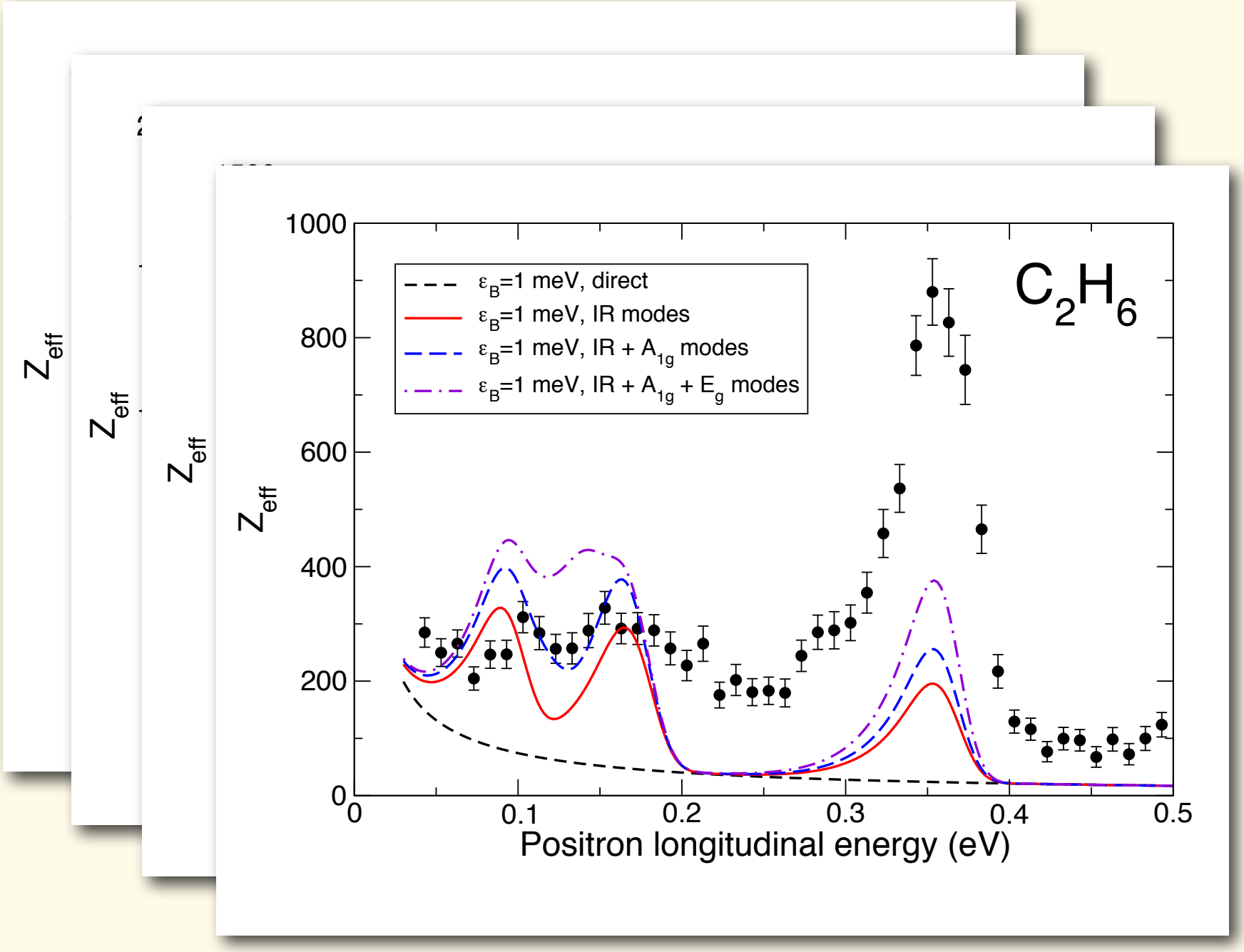

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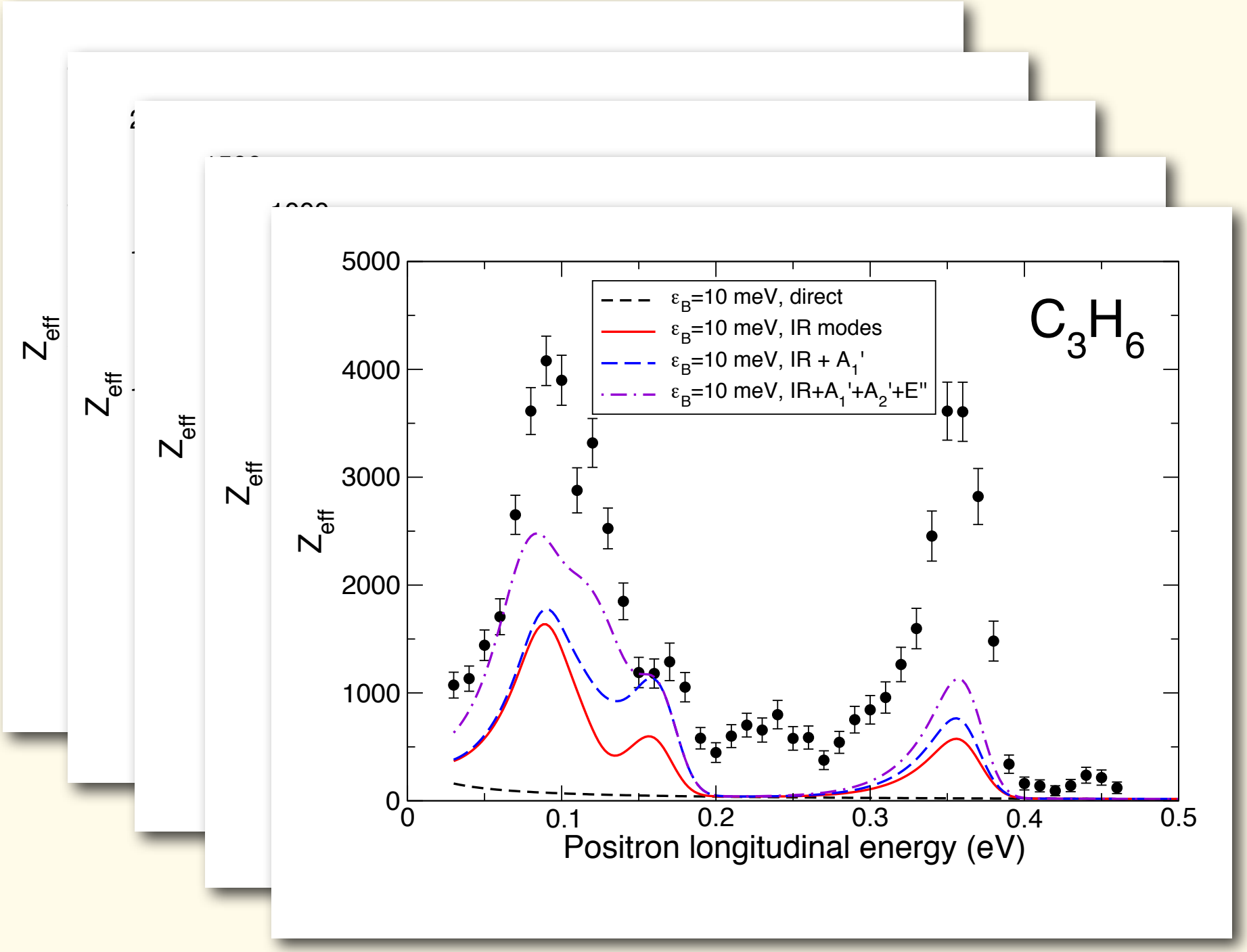

Similarity between $Z_{\rm eff}$ and spectrum of modes

Vibrational modes act as "doorways" into VFR

G. F. Gribakin and P. M. W. Gill, Nucl. Instrum. Methods B **221**, 30 (2004)

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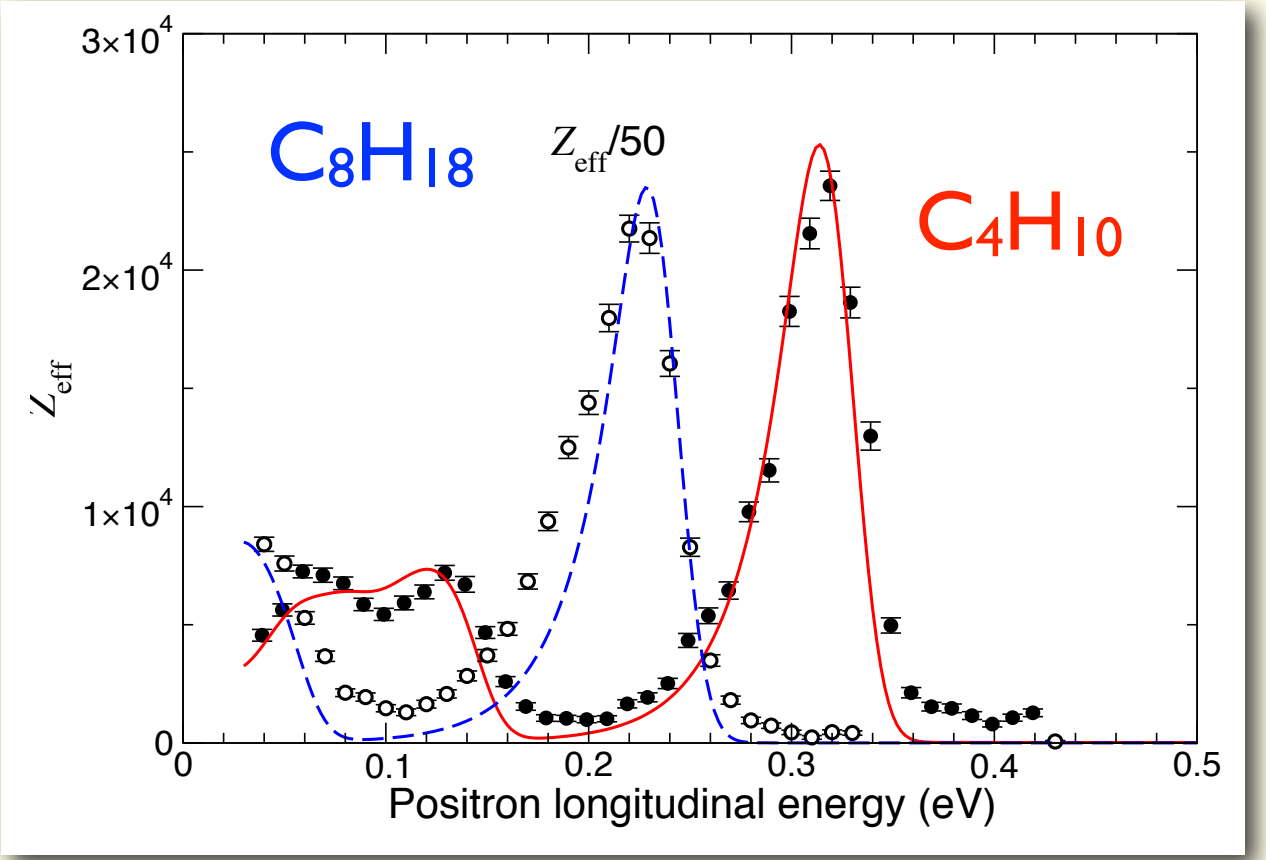
Fit using fixed ratios

Γ_n^e/Γ

for C-H and low-energy modes



Zero-range potential model for positron binding

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Experimental binding energies

No. of C's	BE (meV)	2nd (meV)
3	10	-
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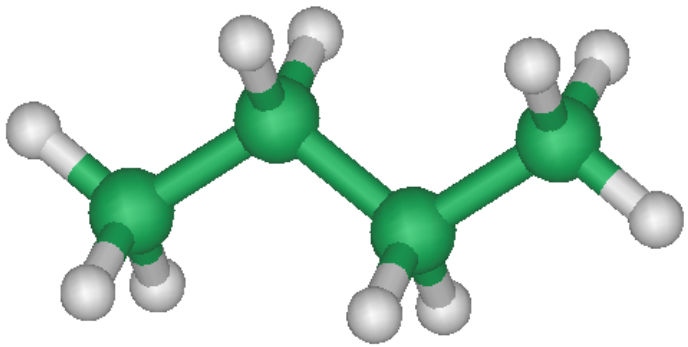
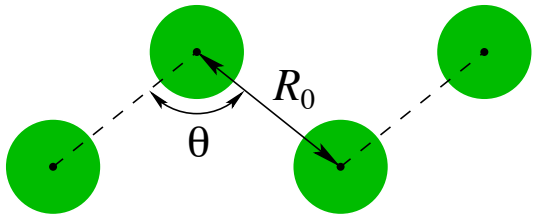


Modelling butane



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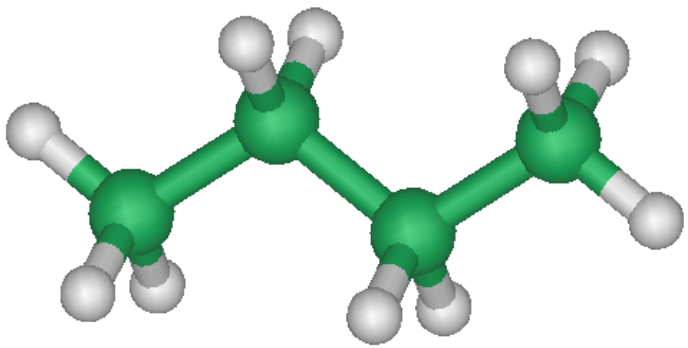

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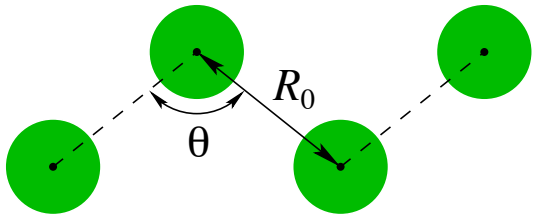
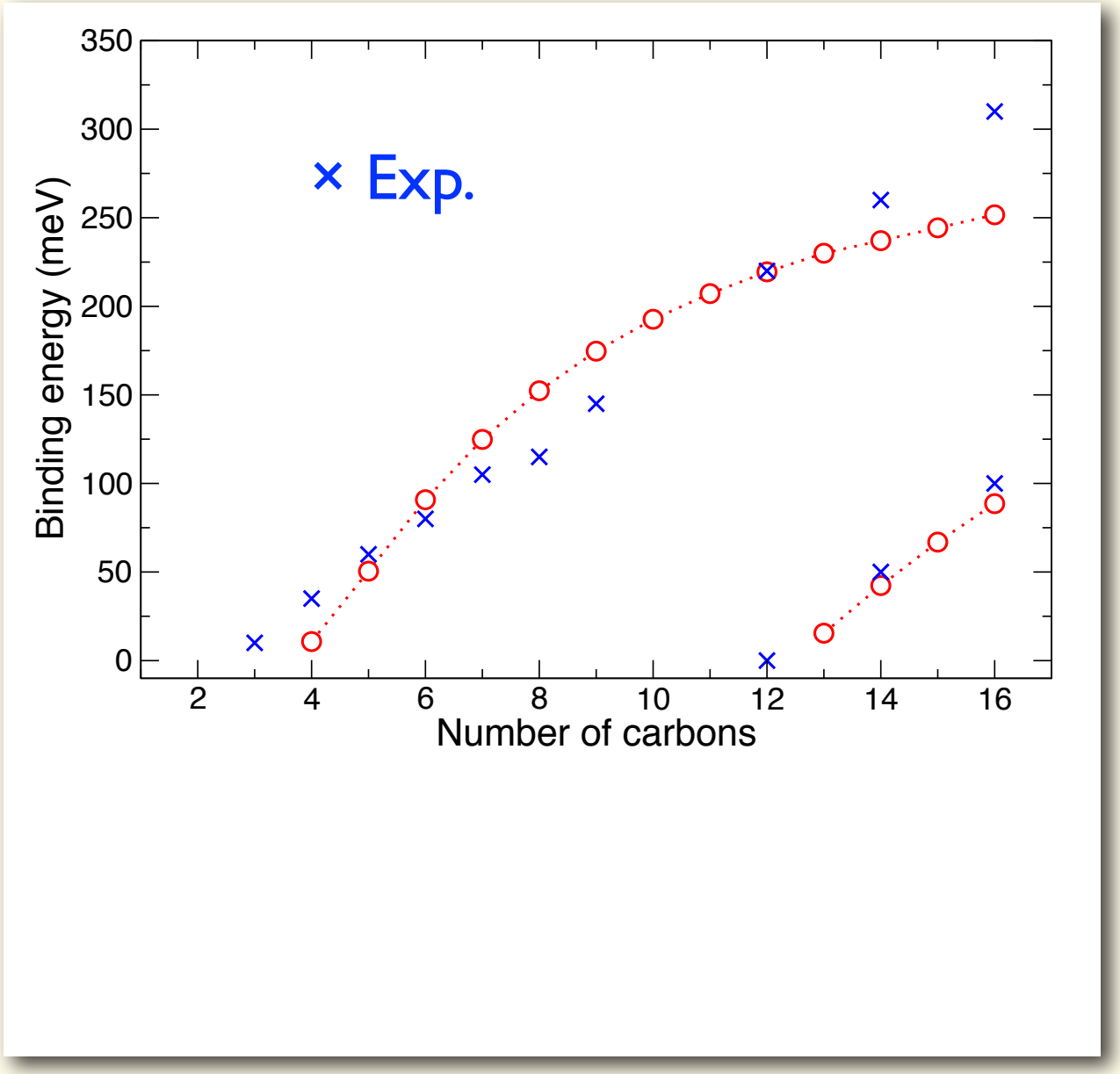


Zero-range wavefunction: $\Psi(\mathbf{r}) = \sum_i A_i \frac{e^{-\kappa|\mathbf{r}-\mathbf{R}_i|}}{|\mathbf{r}-\mathbf{R}_i|}$

Boundary condition: $\Psi|_{\mathbf{r}\to\mathbf{R}_i} \simeq \text{const} \times \left(\frac{1}{|\mathbf{r}-\mathbf{R}_i|} - \kappa_{0i}\right)$

Binding energies for alkanes: theory vs experiment



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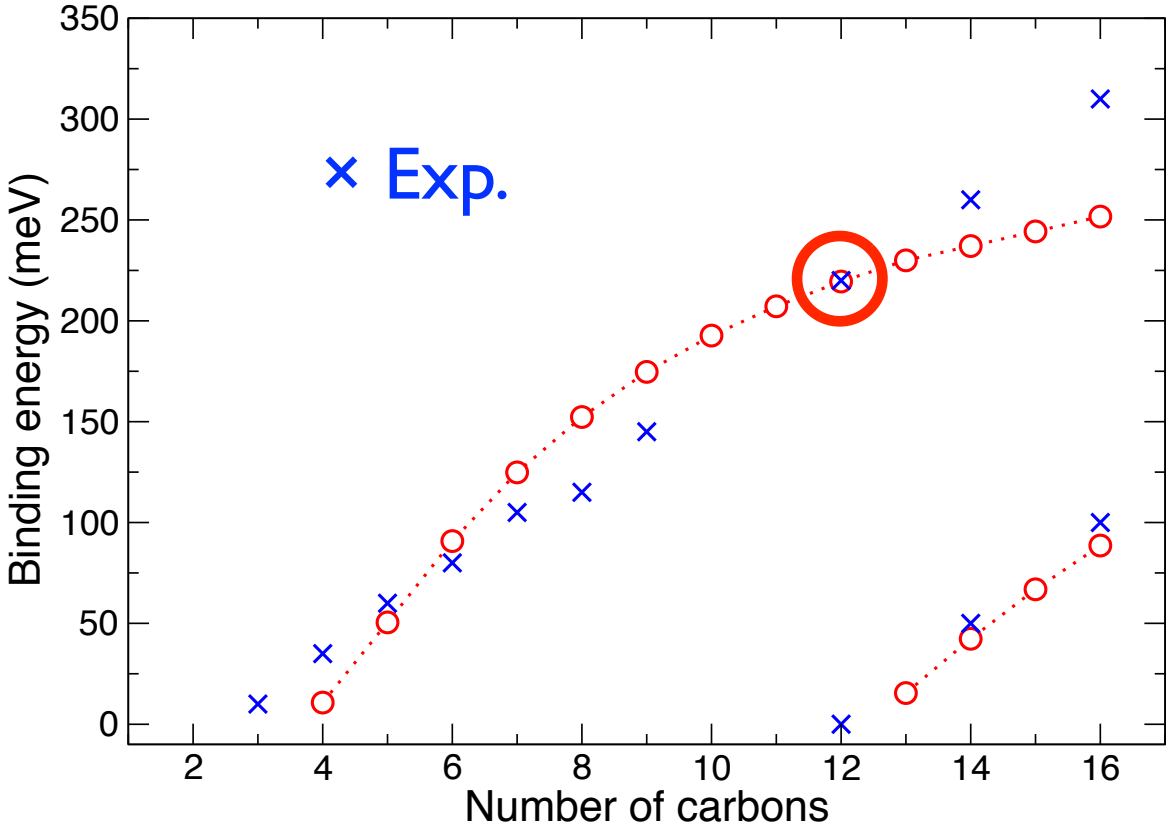

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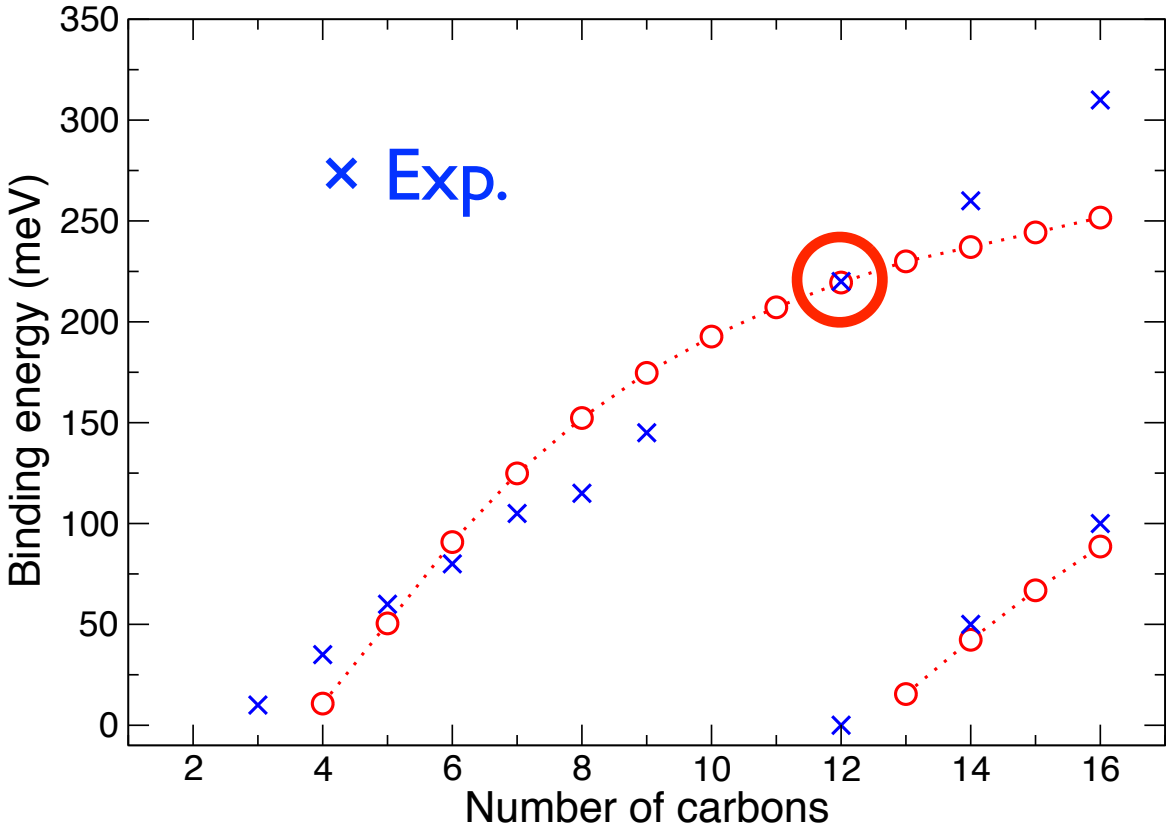

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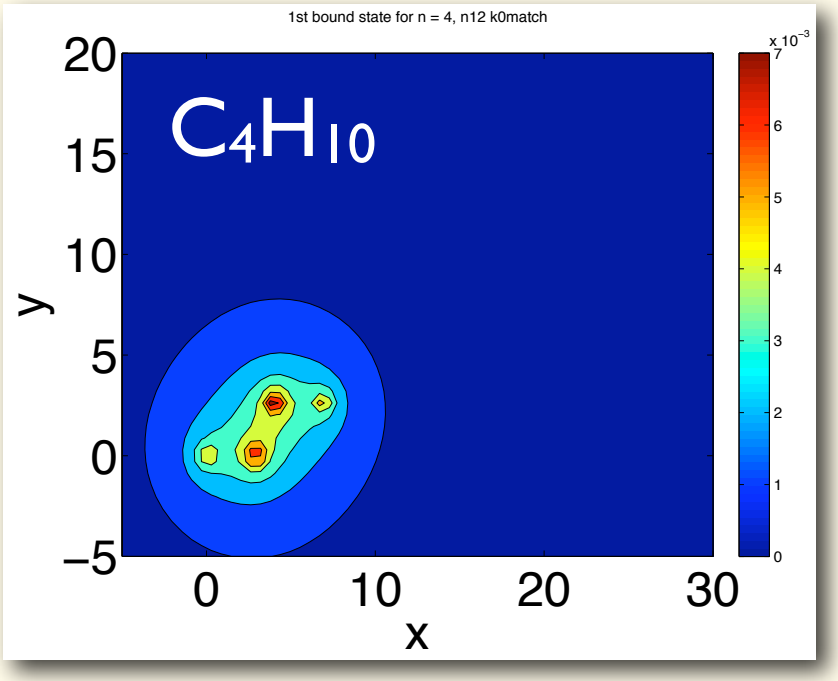
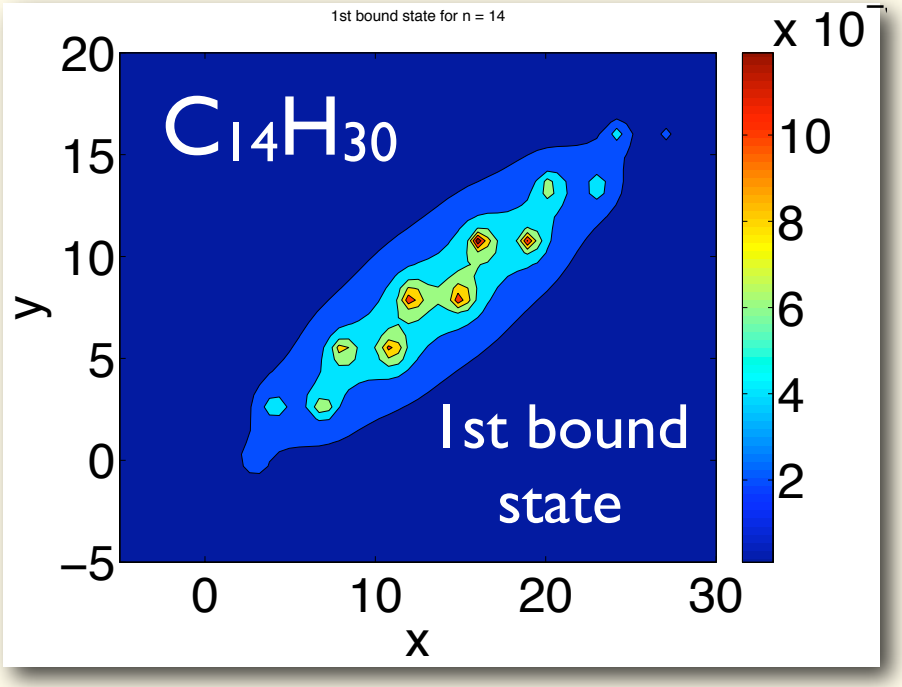
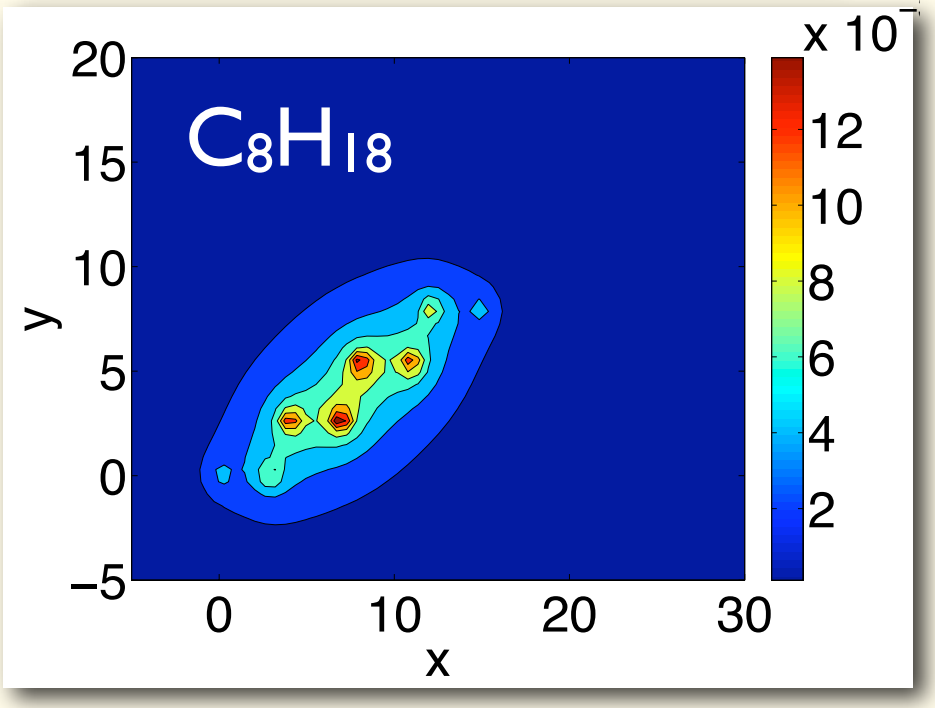
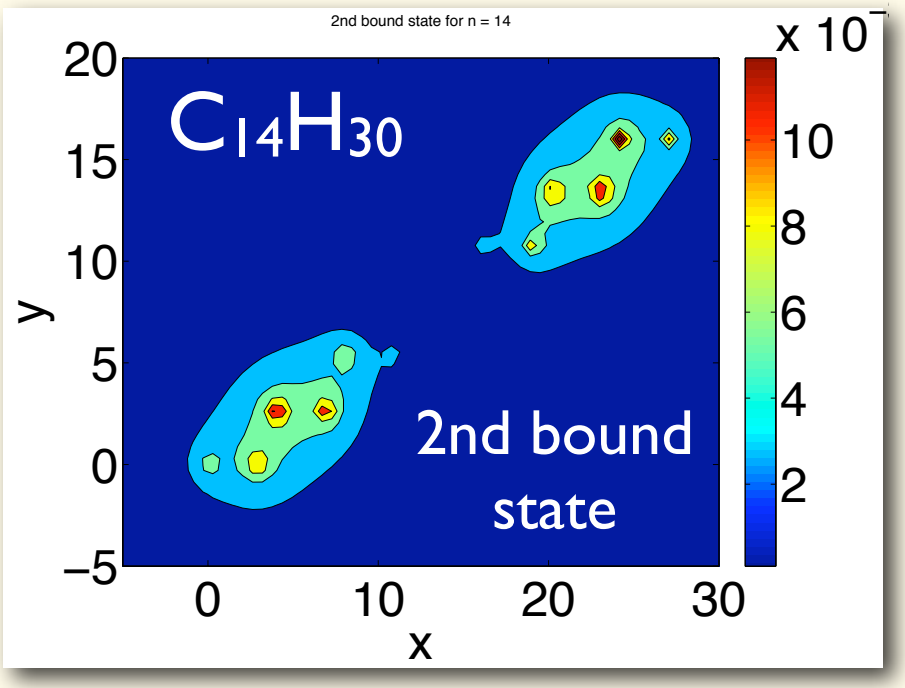
Theory predicts emergence of the 2nd positron bound state!

2D density of the bound states









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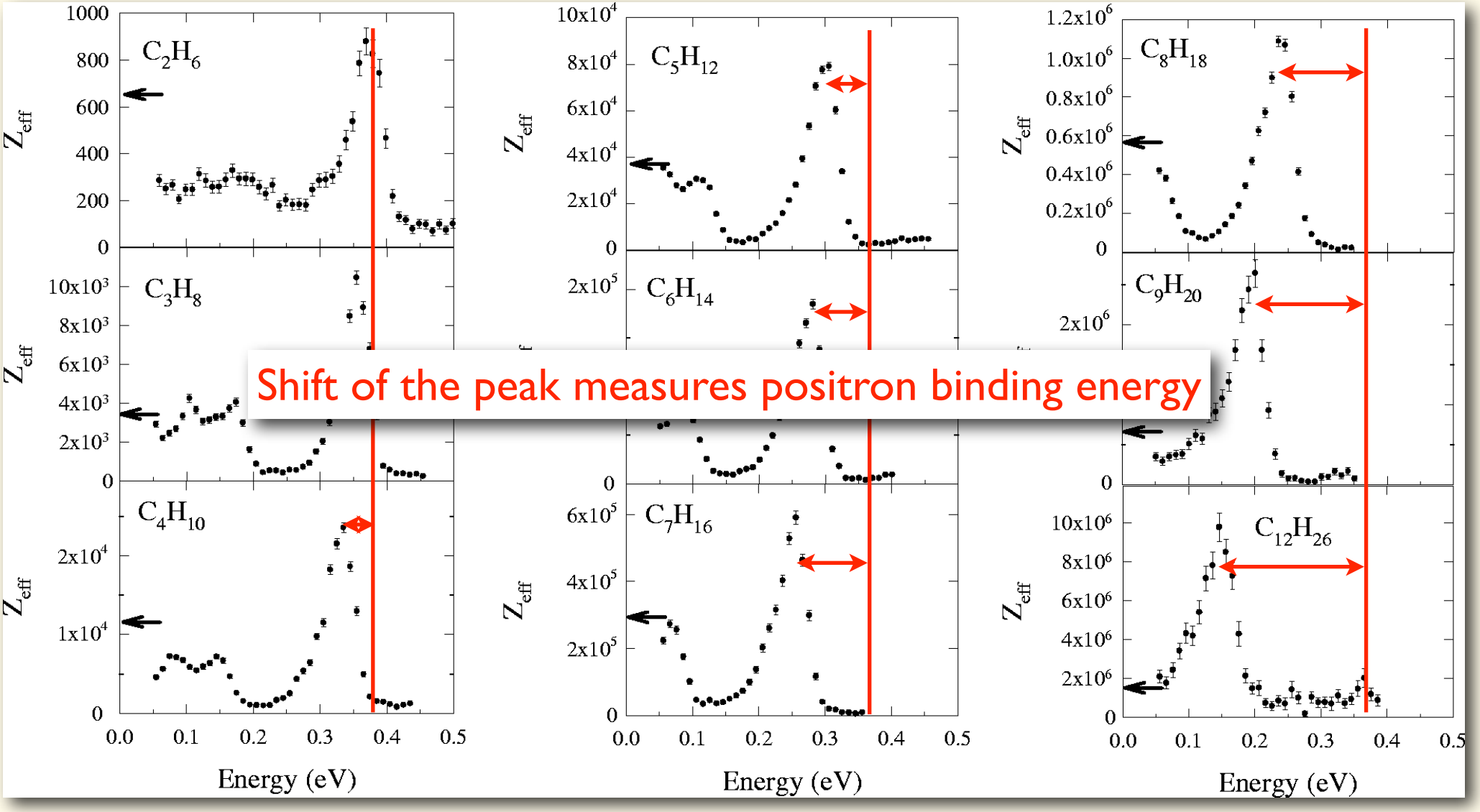

C-H vibrational mode $\omega \approx 0.37$ eV

Barnes et al. PRA **67**, 032706 (2003)

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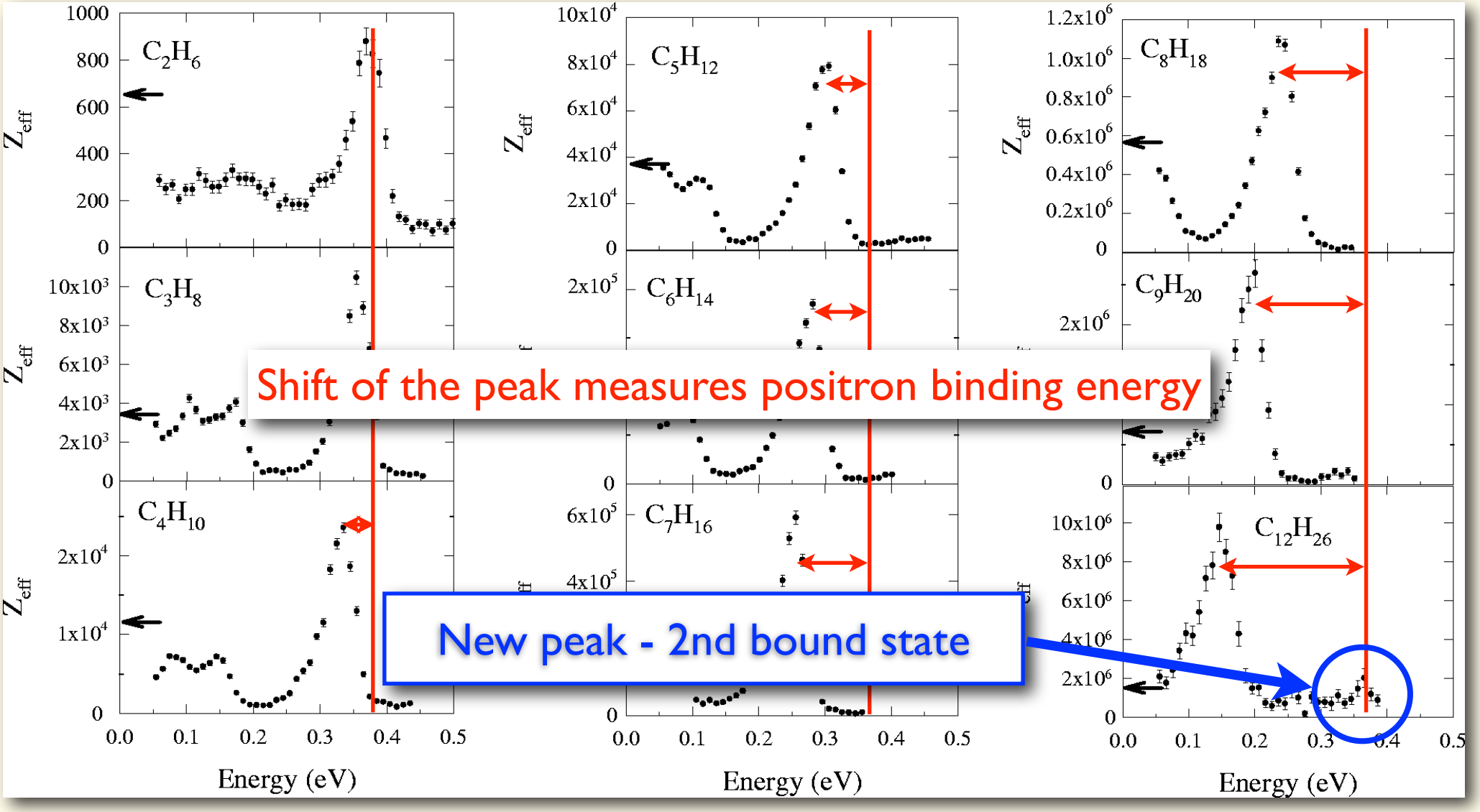

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Open questions

- Positron binding to open-shell atoms?
- Positron-atom electronic Feshbach resonances?
- Positron binding to nonpolar molecules?
- Positron annihilation rates in molecular bound states?
- Positron coupling to non-IR-active vibrations?
- Quantitative description of enhancement of resonances due to vibrational mode coupling (IVR)?

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THANK YOU