42nd Polish Seminar on Positron Annihilation

Lublin, 29 June - 1 July 2015

Towards matching between positron scattering in gas-phase and positron annihilation in condensed phase

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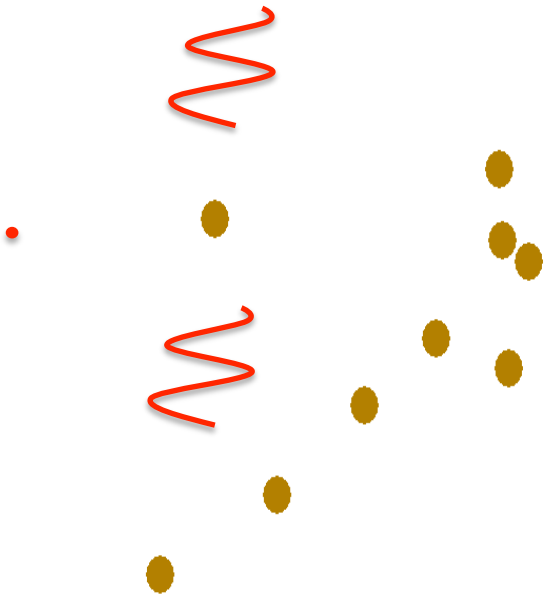
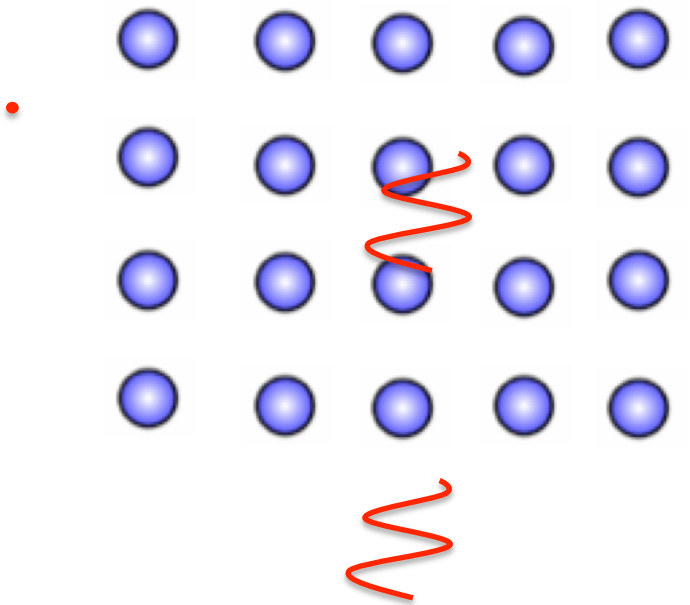
Binary and multibody interactions

positron – gas interaction

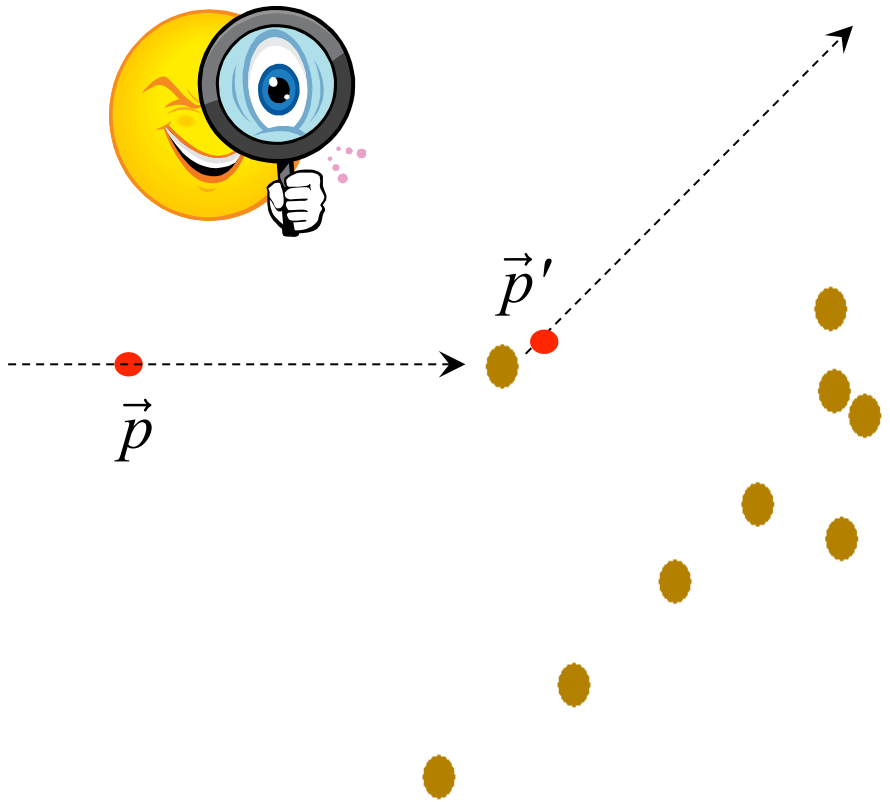


positron – condensed matter interaction



One of the objectives of our study is to find any qualitative or quantitative links between low-energy positron interaction with the matter in gas and condensed phases – regarding also the annihilation process.

Positron – gas interaction
scattering channels



$p = p'$

- elastic scattering
- virtual positronium?

$p \neq p'$

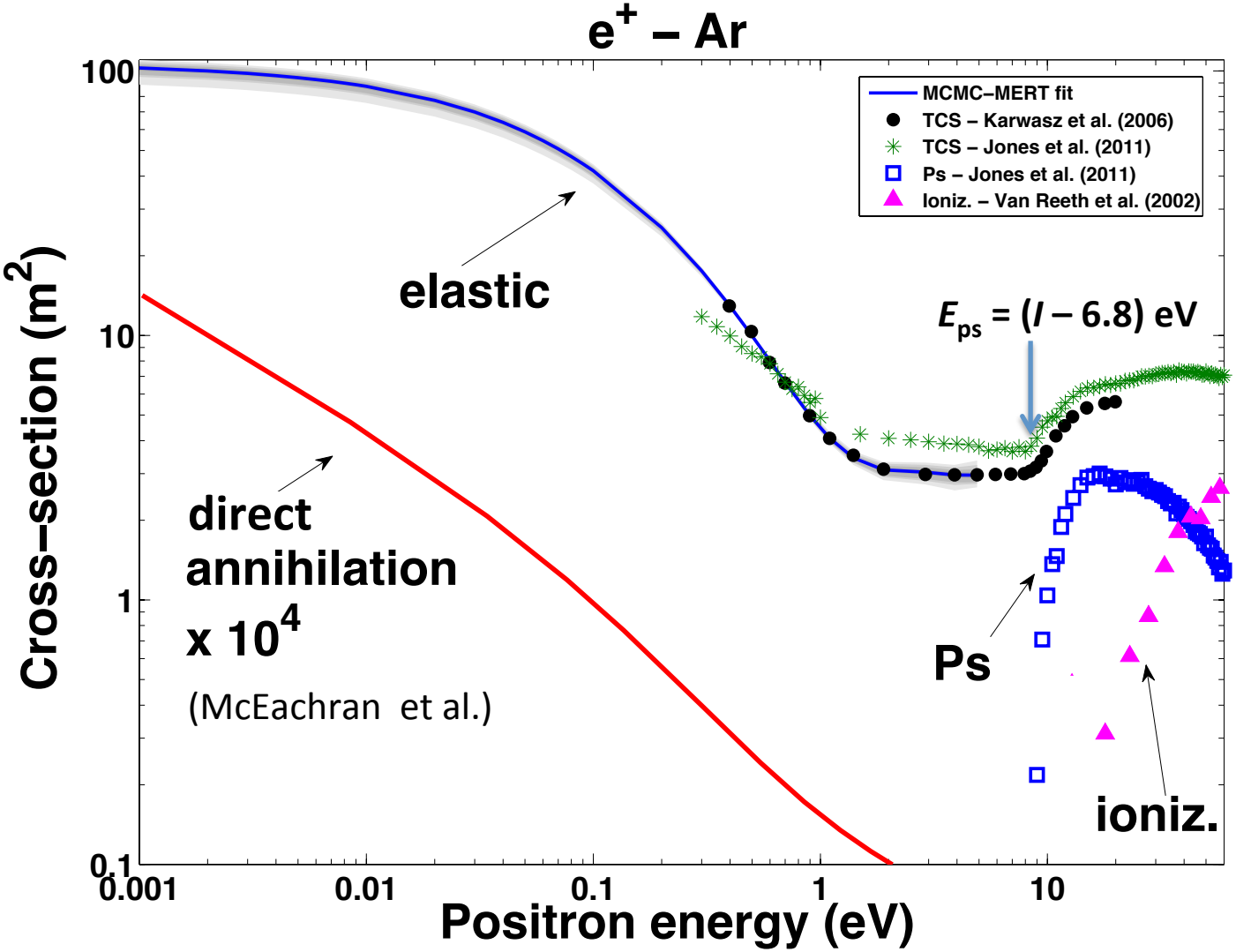
- rotational, vibrational or electronic excitation
- ionization

➢ positronium formation

➢ direct annihilation (2γ or 3γ)

Cross - sections

Total cross-sections = the overall probablility of a single positron scattering (sum over all active scattering channels)

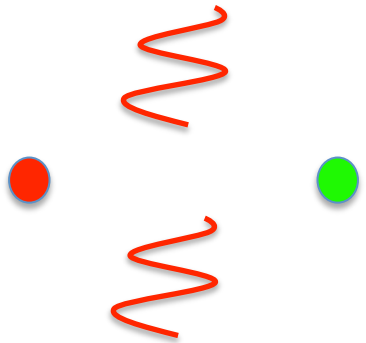


Cross-sections and annihilation rates

For slow positrons $v << c$:

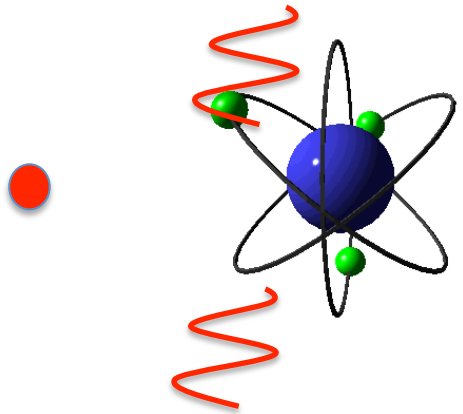
$$\sigma_{ann} = \frac{\pi r_0^2 c}{v}$$

free positron – electron annihilation



$$\sigma_{ann} = \frac{\pi r_0^2 c}{v} Z$$

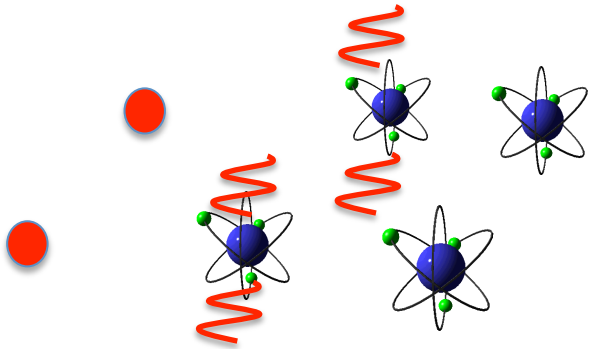
positron – atom annihilation (*Z bound* electrons)



$$\lambda = \sigma_{\text{ann}} v n = \pi r_0^2 c Z n$$

annihilation rates

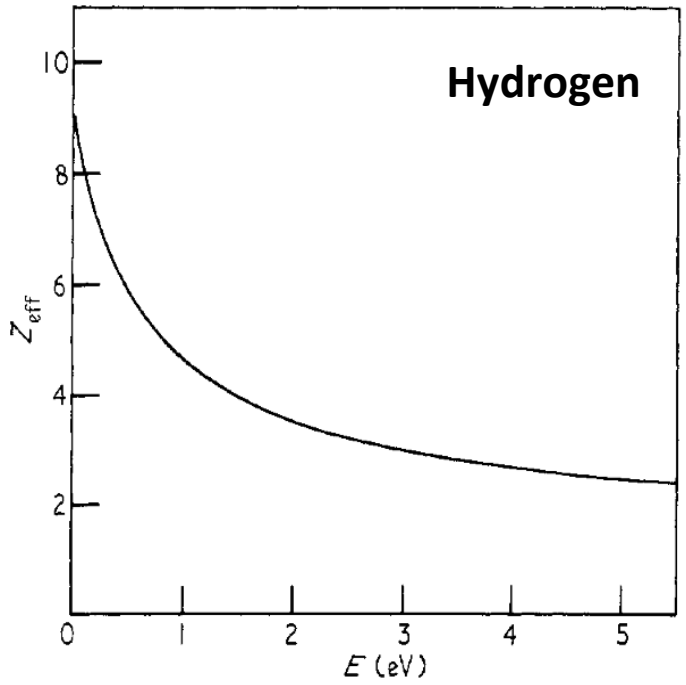
= number of events per second



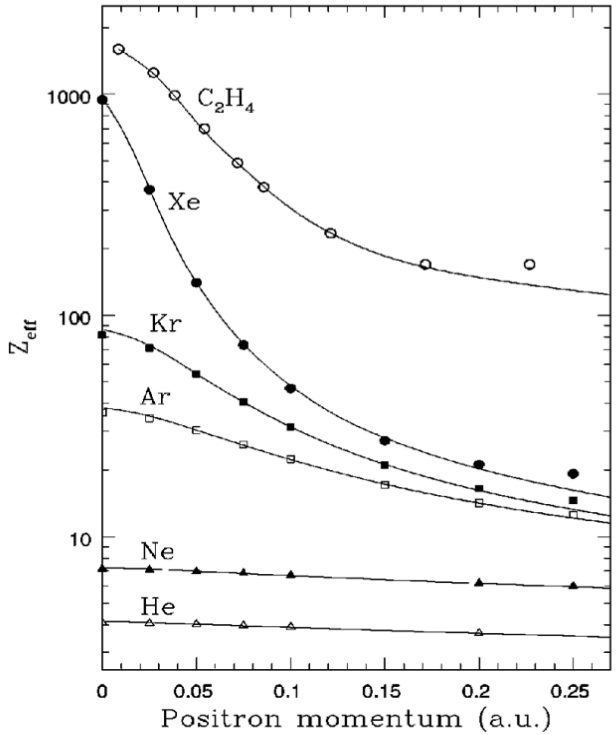
Z_{eff} – effective electron number

Z_{eff} can interpreted as a measure of the probability of the positron being at the same position as any one of the electrons in the target and it can be calculated from the total positron-atom scattering wave function

$$Z_{\text{eff}} = Z\int\left|\Psi\left(\vec{r}_p,\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_z\right)\right|^2\delta\left(\vec{r}_p-\vec{r}_i\right)d\vec{r}_p\,d\vec{r}_1\,d\vec{r}_2\ldots\vec{r}_Z$$



Humberston and Wallace, J. Phys. B **5**, 1138 (1972)



Gribakin, Phys. Rev. A **61**, 022720 (2000)

Deformation of electronic cloud:

- **long-range dipole interaction**
- short-range correlation effects

Induced-dipole polarization effect on elastic scattering cross-section

PHYSICAL REVIEW A **88**, 012704 (2013)

Analytic approach to modified effective-range theory for electron and positron elastic scattering

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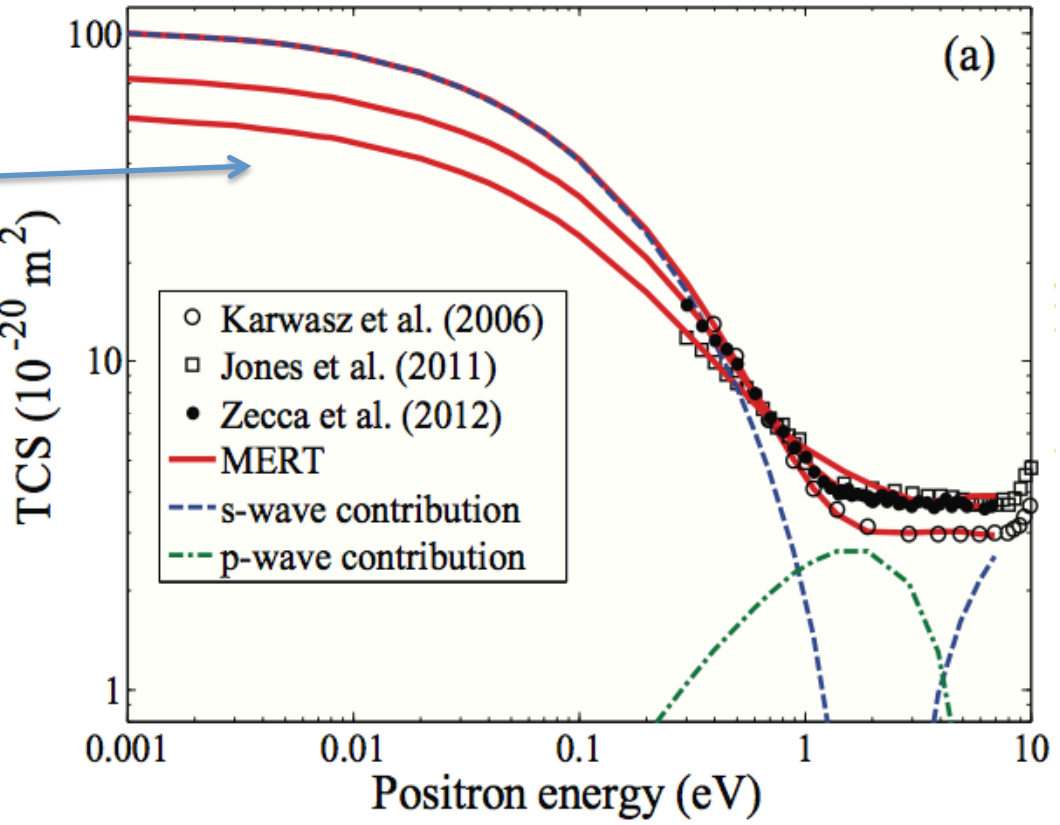
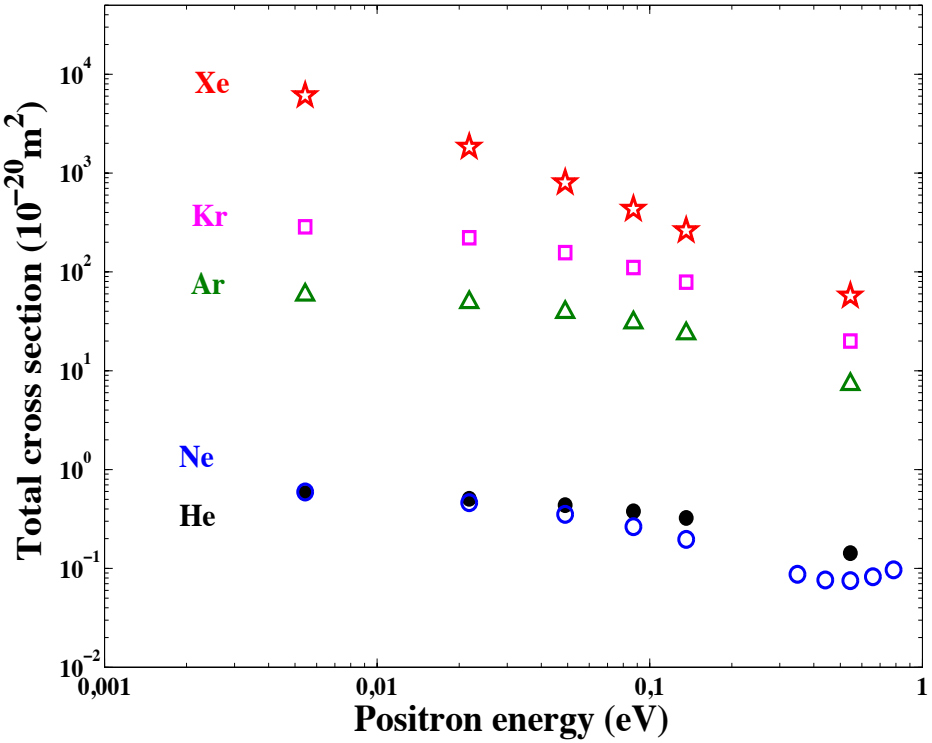
(Received 6 May 2013; published 8 July 2013)

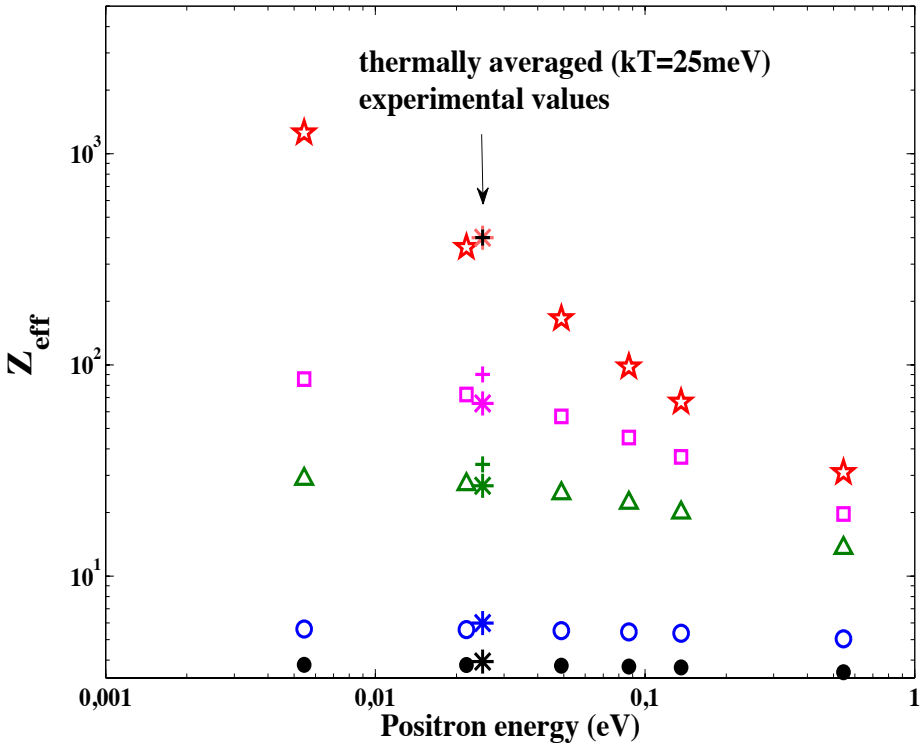
enhancement due to the attractive induced-dipole polarization interaction



Positron direct annihilation vs elastic scattering cross-section

low-pressure noble gases at room temperature





***ab-initio* many body calculations by:**

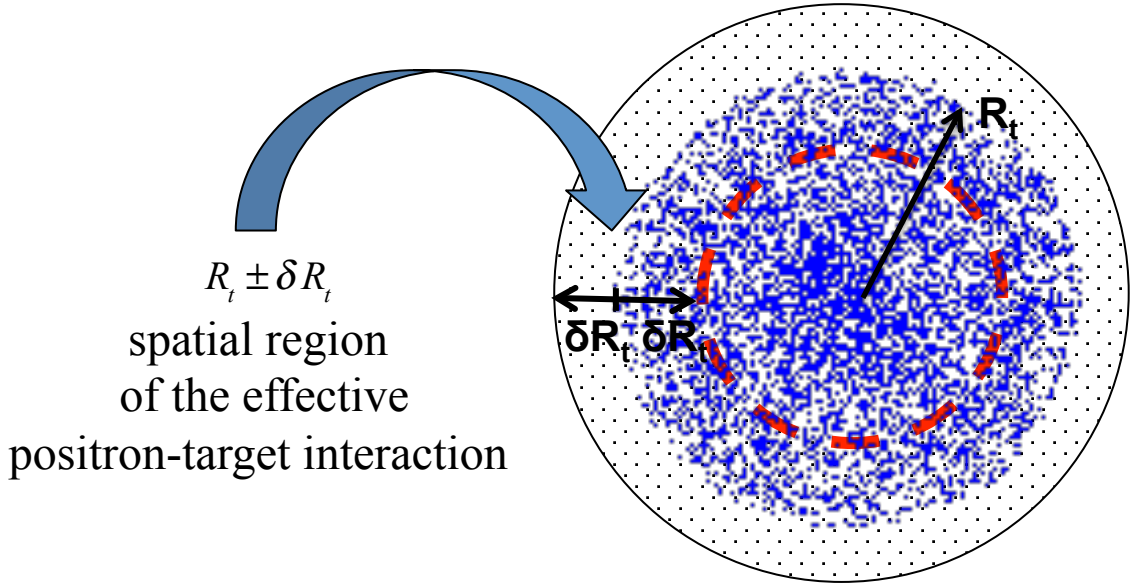
D. G. Green, J. A. Ludlow and G. F. Gribakin, Phys. Rev. A 90, 032712 (2014)

Positron direct annihilation vs elastic scattering cross-section

At low energies Z_{eff} can be modeled by the following relation:

$$Z_{eff}(E) = F\left(R_t^2 + \frac{\sigma_{el}(E)}{4\pi} + \frac{R_t}{k}\sin\left[2\eta_0(E)\right] \right)$$

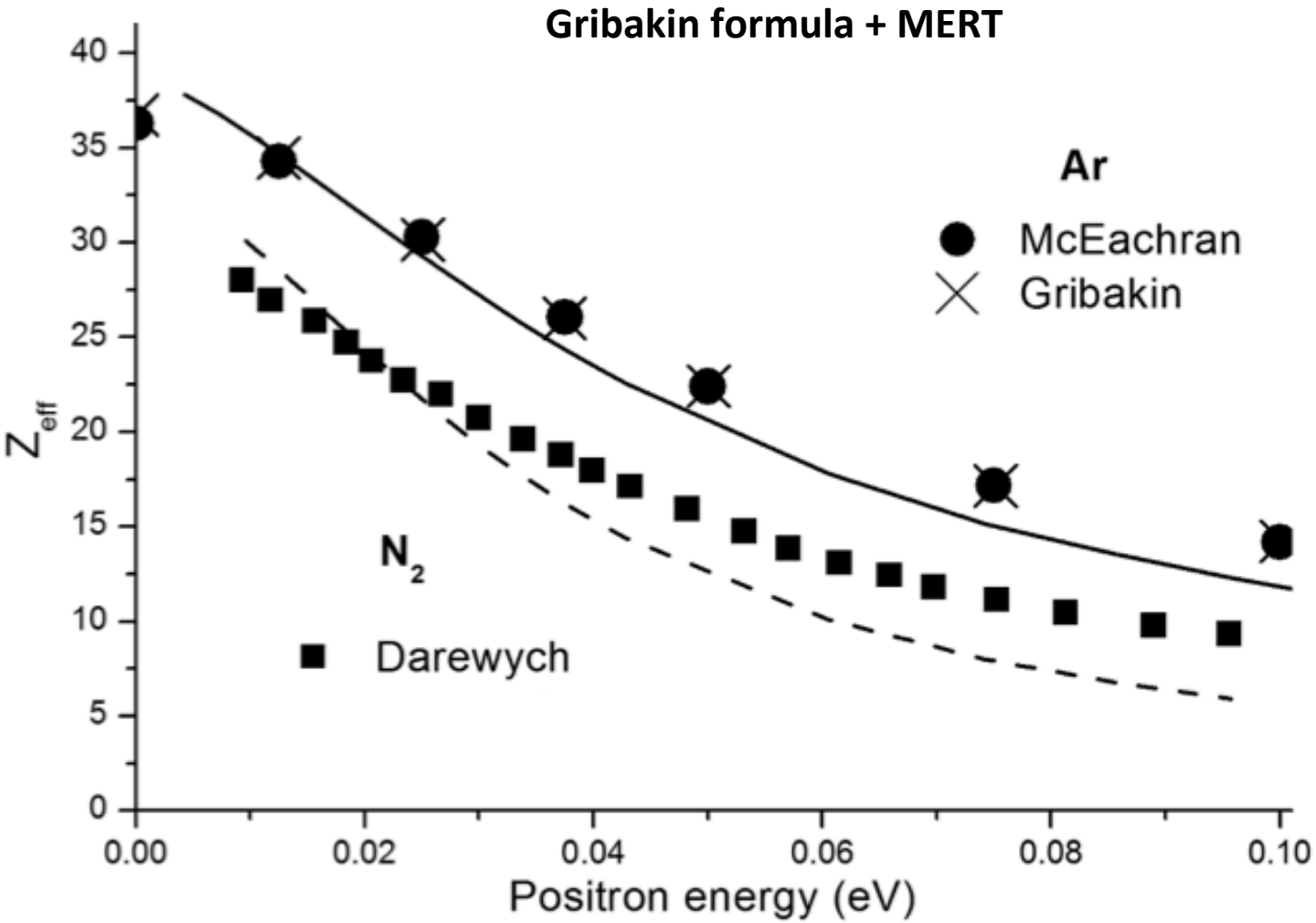
G. F. Gribakin, Phys. Rev. A 61, 022720 (2000)



σ_{el} - elastic scattering cross section

η_0 - *s*-wave scattering phase-shift

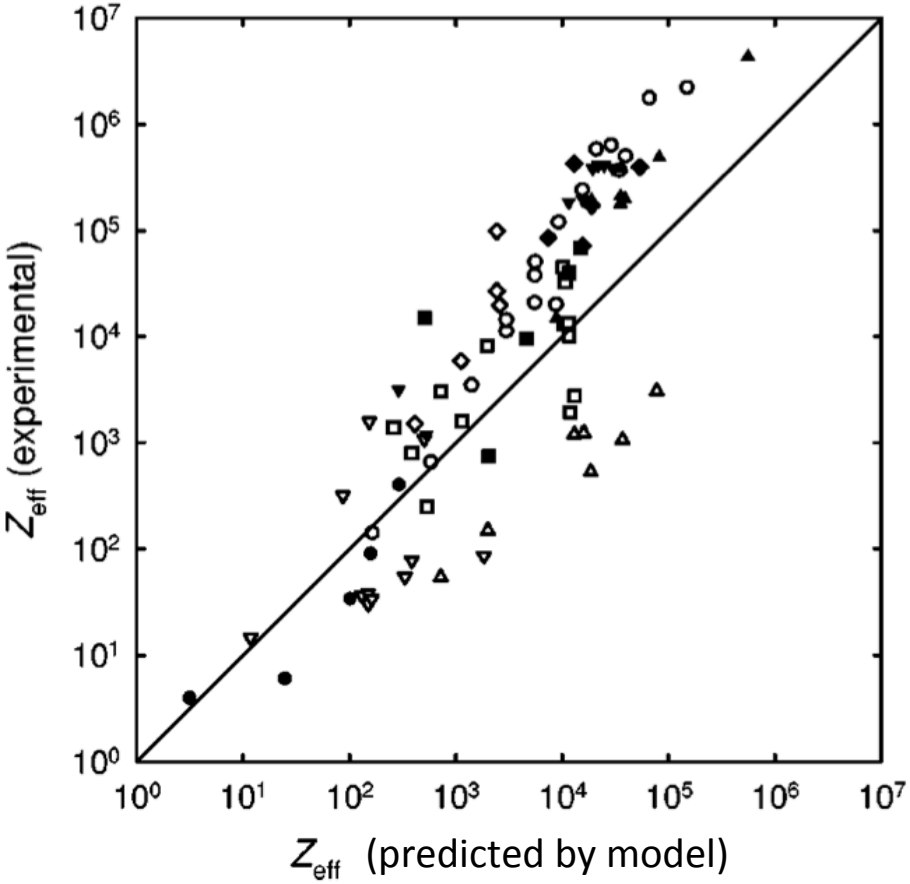
Direct annihilation at low energies in binary collisions



Fedus and Karwasz, Acta Physica Polonica (2013)

Virtual positronium

G. Laricchia and C. Wilkin, Phys. Rev. Lett. 79, 2241 (1997)



(●) noble gases, (∨) inorganic molecules, (○) alkanes, (solid triangle, down) alkenes and acethylene, (solid triangle, up) aromatic hydrocarbons, (△) perfluorinated alkanes, (solid square) perchlorinated alkanes, CBr_4, CH_3Cl, and CCl_2F_2, (◇) alchohols, carboxylic acids, ketones, (solid diamond) substituted benzenes, and (□) partially fluorinated hydrocarbons. (—) is the line $y = x$.

The virtual positronium can be formed for a time interval:

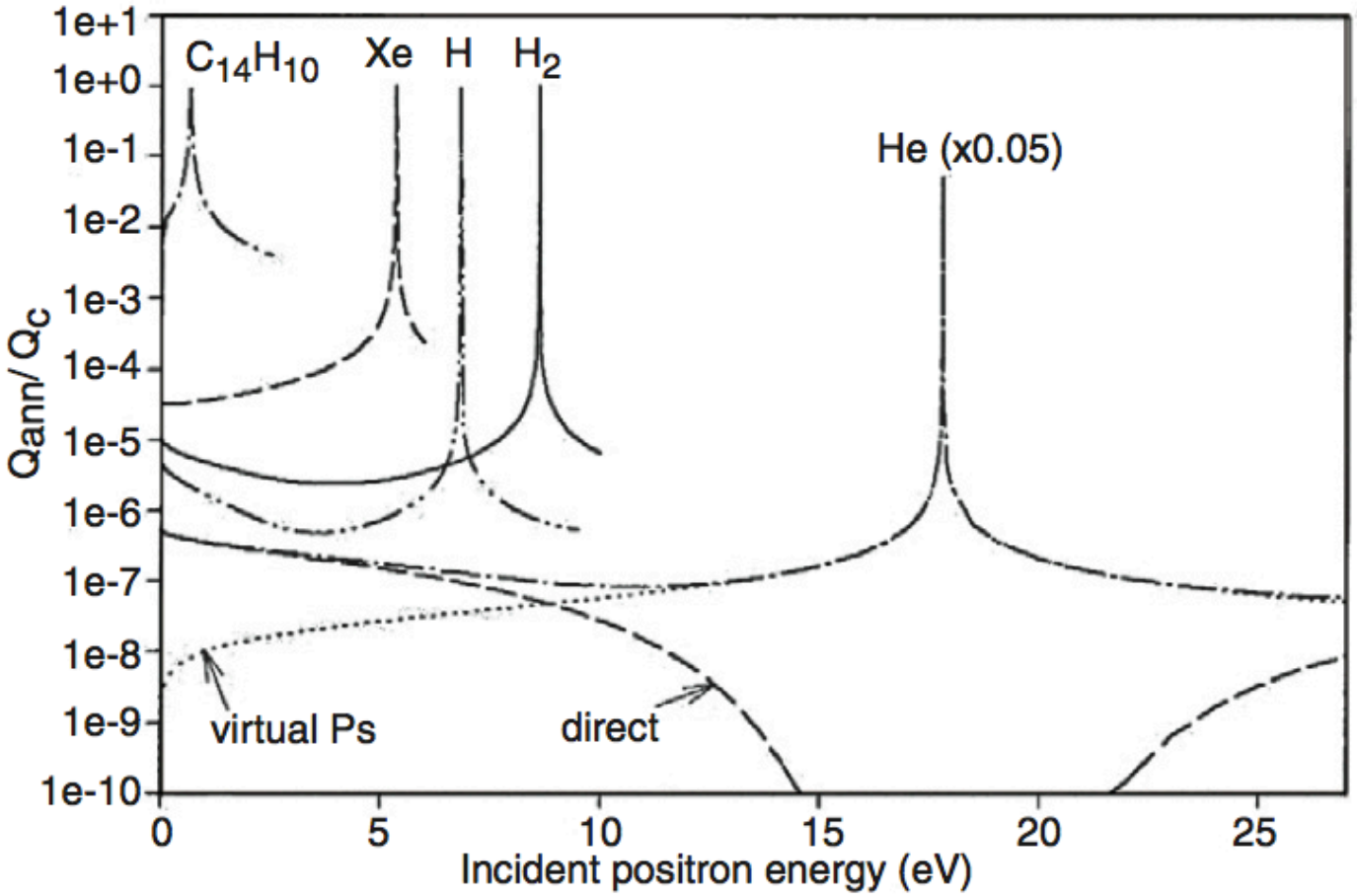
$$\Delta t = \frac{\hbar}{\left| E - I - E_{ps} \right|}$$

The total annihilation rate to be the sum of direct annihilation and the annihilation of virtual positronium due to ''self'' and ''pickoff'' annihilation.

$$Z_{\text{eff}} = \frac{\sigma v}{\pi r_0^2 c}\{\gamma[1 - \exp(-\lambda\tau)] + (1-\gamma) \times [1 - \exp(-\Delta t(\lambda_{sa} + \lambda_{po}))]\},$$

Direct annihilation vs virtual positronium annihilation

Qualitative energy dependence of the ratios of the annihilation cross- section (Q_{ann}) to the collision cross-section (Q_c)



G. Laricchia and C. Wilkin, Phys. Rev. Lett. 79, 2241 (1997)

Van Reeth et al., Physica Scripta, 71 C9 (2005)

Virtual positronium contribution to elastic scattering cross-section

PHYSICAL REVIEW A **90**, 032712 (2014)

Positron scattering and annihilation on noble-gas atoms

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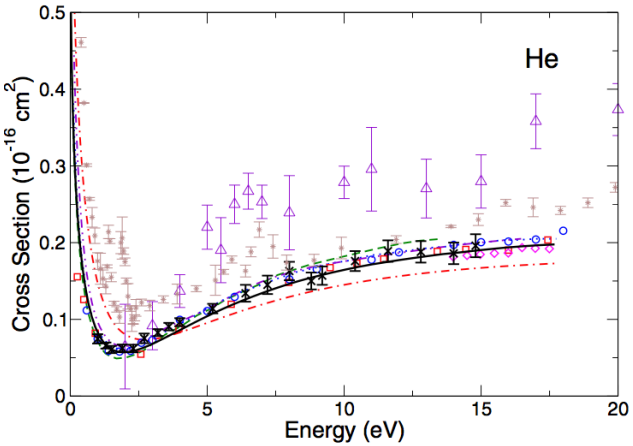
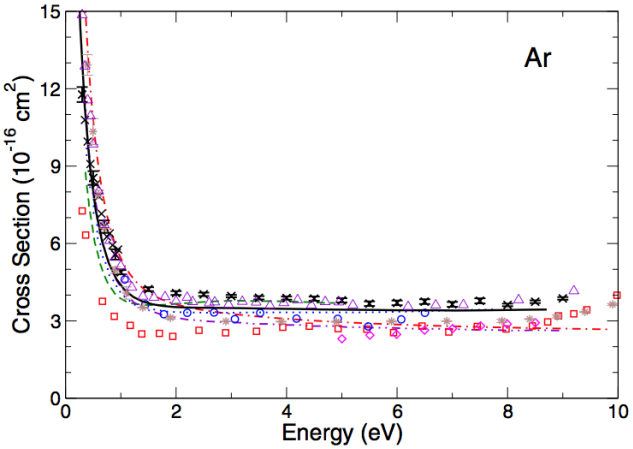
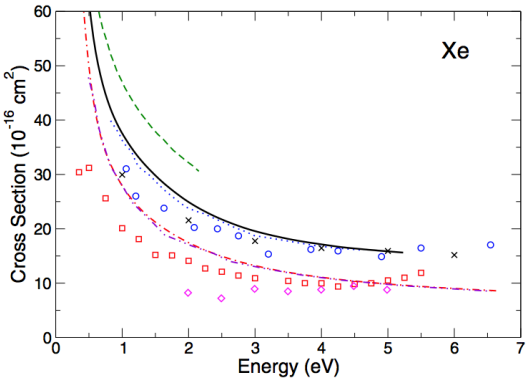
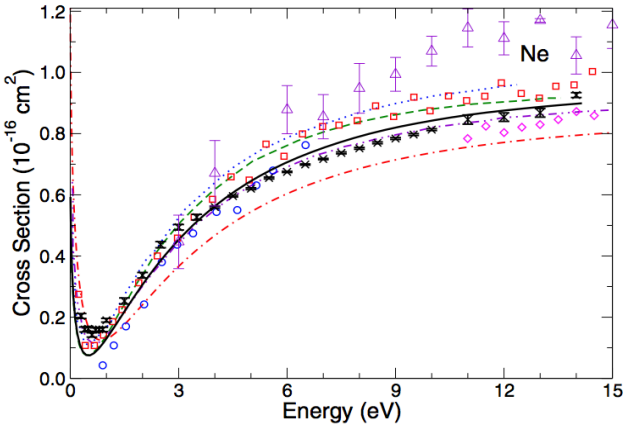
Department of Applied Mathematics and Theoretical Physics, Queen's University Belfast, Belfast BT7 1NN, Northern Ireland, United Kingdom

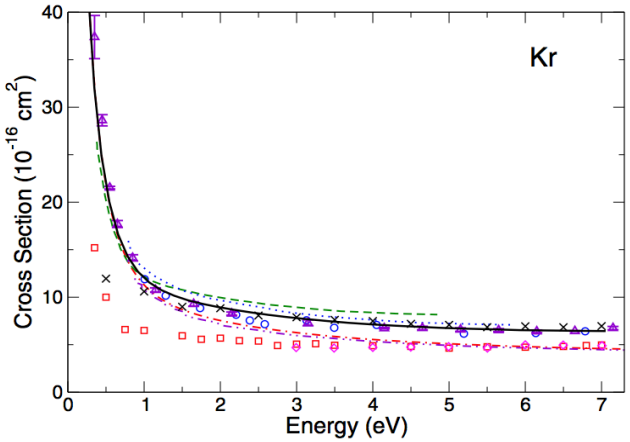
(Received 31 July 2014; published 10 September 2014)







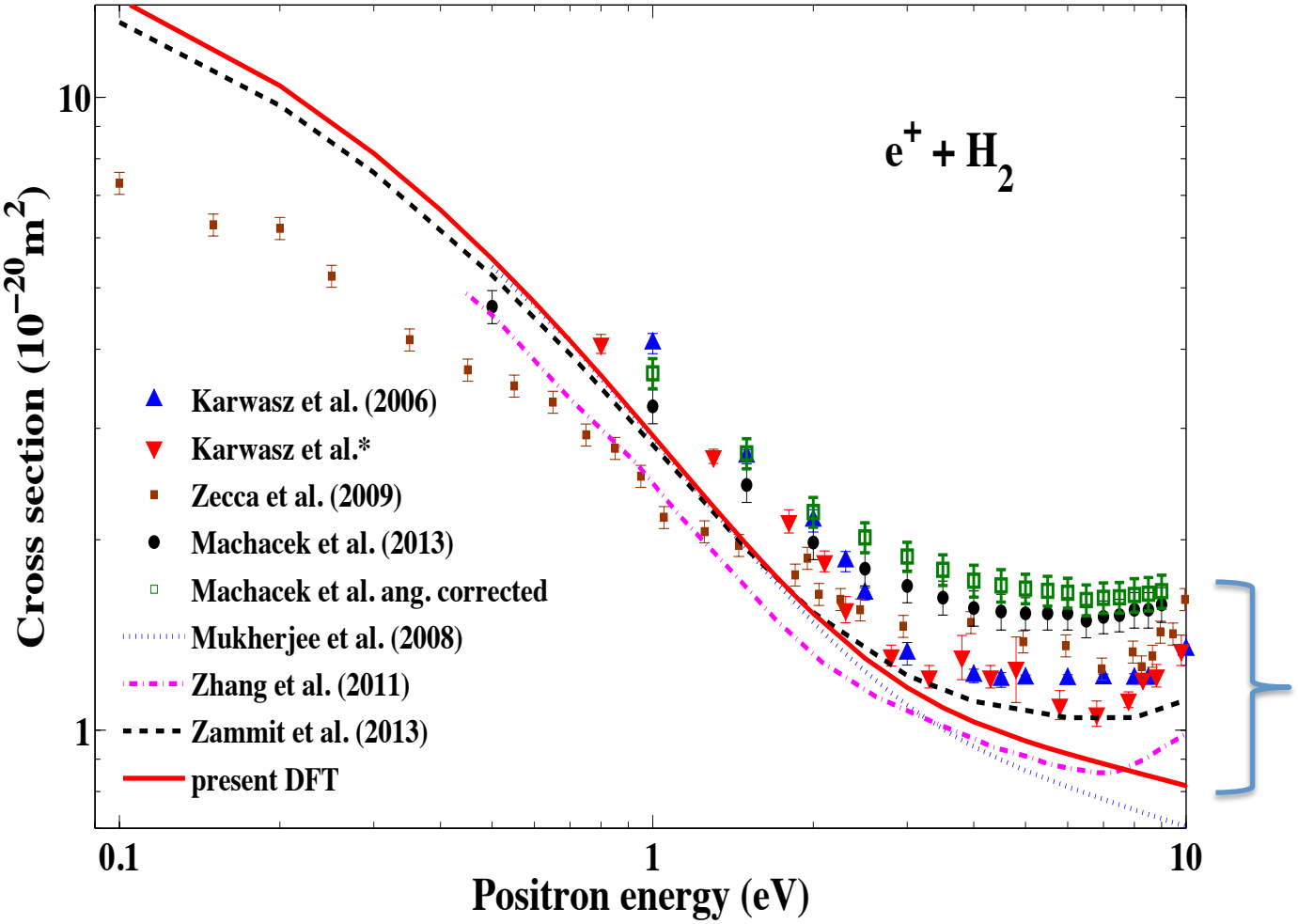




PHYSICAL REVIEW A **91**, 062701 (2015)

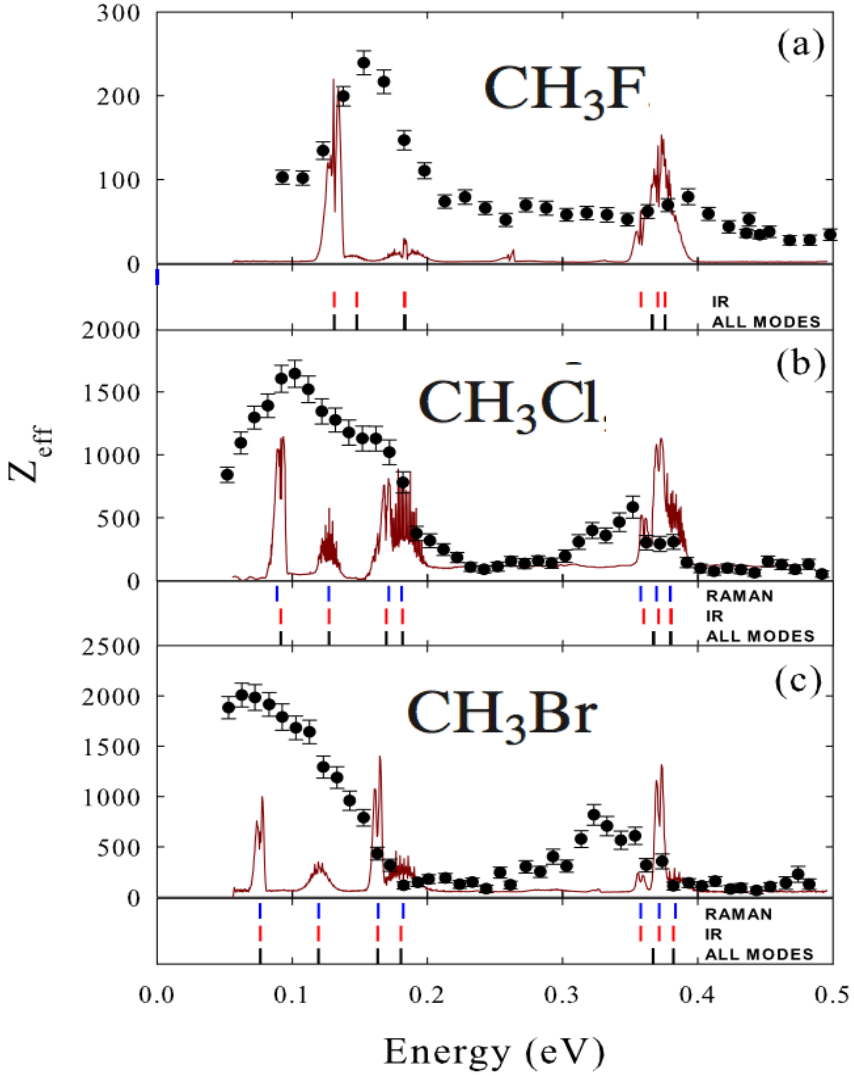
Positron scattering on molecular hydrogen: Analysis of experimental and theoretical uncertainties

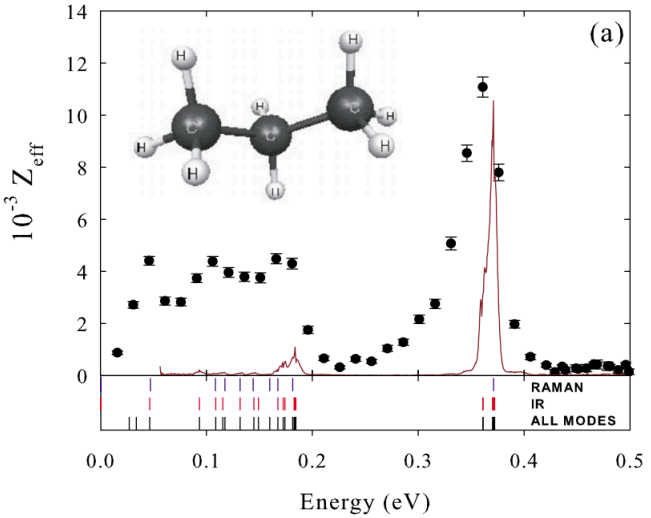
Kamil Fedus,[1,*] Jan Franz,[2,†] and Grzegorz P. Karwasz[1,‡]

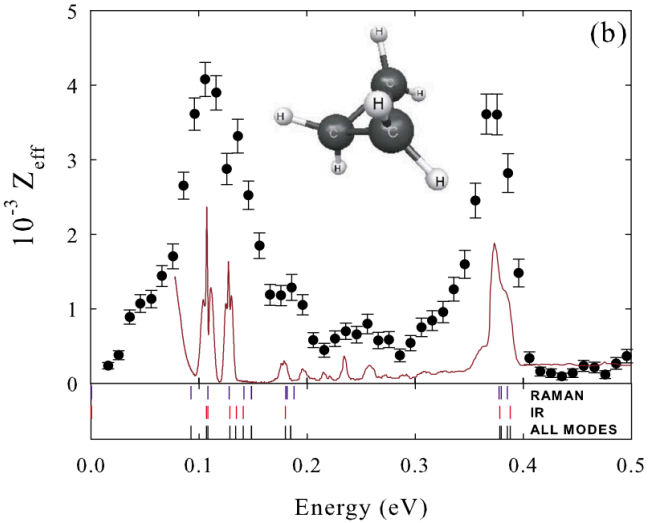


virtual positronium?

Significant enhancement of annihilation rate in large molecular systems





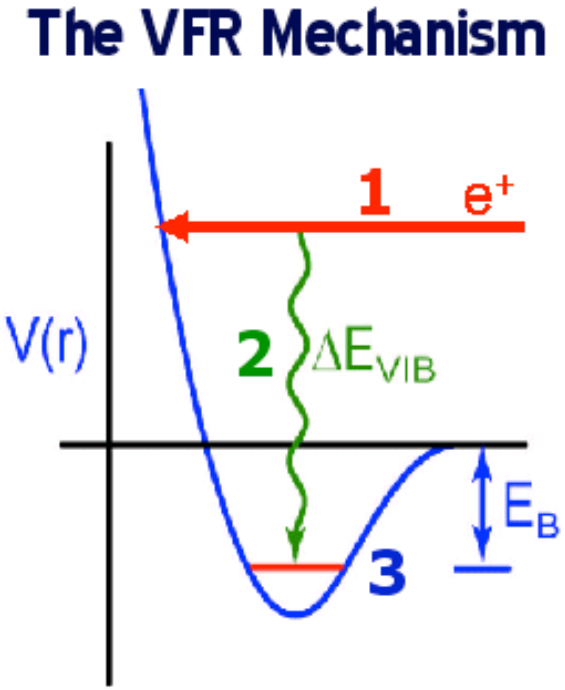


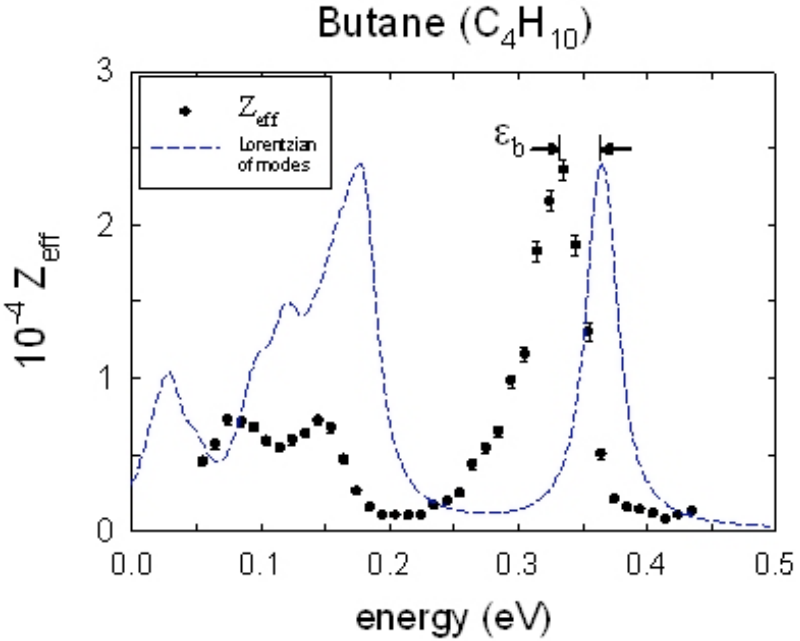
Cliff Surko website: https://physics.ucsd.edu/research/surkogroup/

Vibrational Feschbach Resonance (VFR)

Resonance in annihilation can be described by a vibrational Feshbach resonance (VFR) mechanism:

1. A positron approaches the molecule with the resonant energy ($E = \Delta E_{VIB} + \varepsilon_B$)
2. The positron transfers its energy into a molecular vibration of energy ΔE_{VIB} and drops into a bound state of depth ε_B
3. In this state, the positron wavefunction strongly overlaps the electron wavefunction resulting in enhanced probability of annihilation.

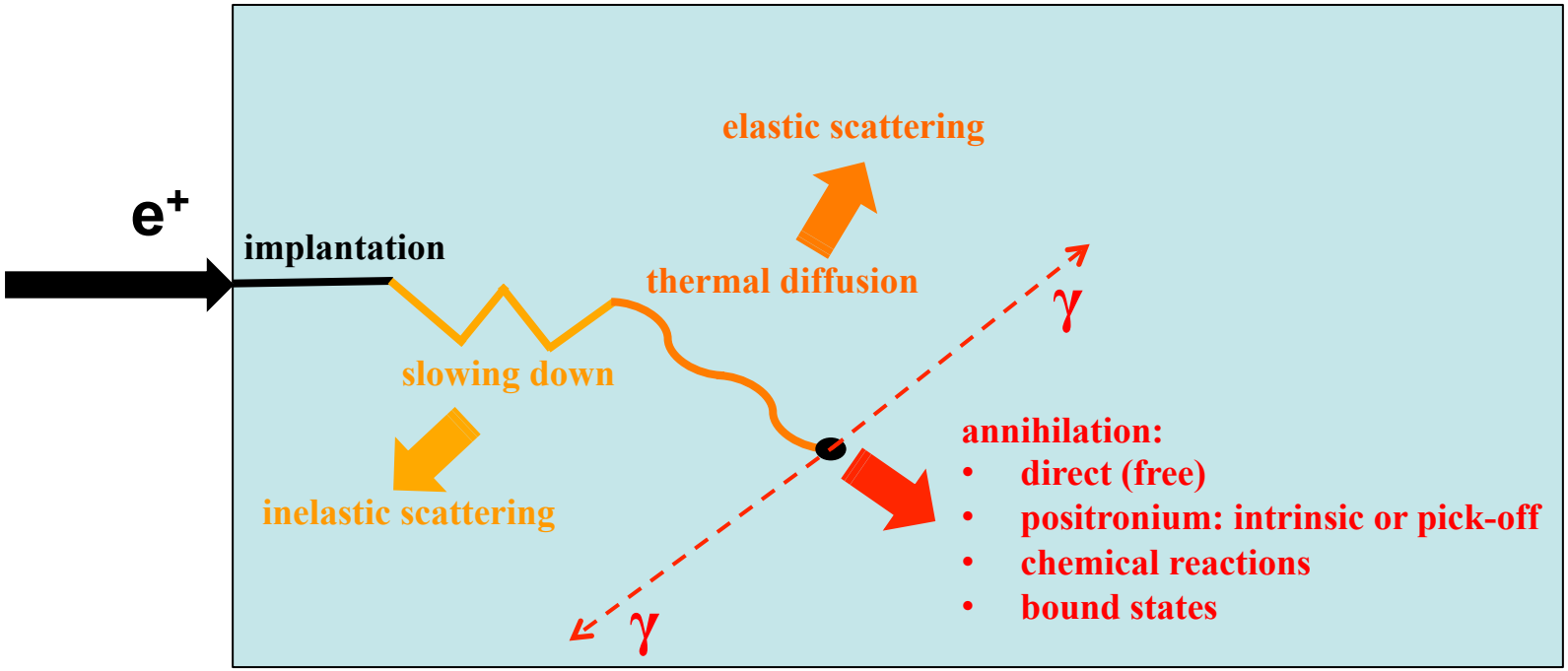




In this interpretation, each Z_{eff} peak is shifted below a vibrational mode by the binding energy ε_B.

Cliff Surko website: https://physics.ucsd.edu/research/surkogroup/

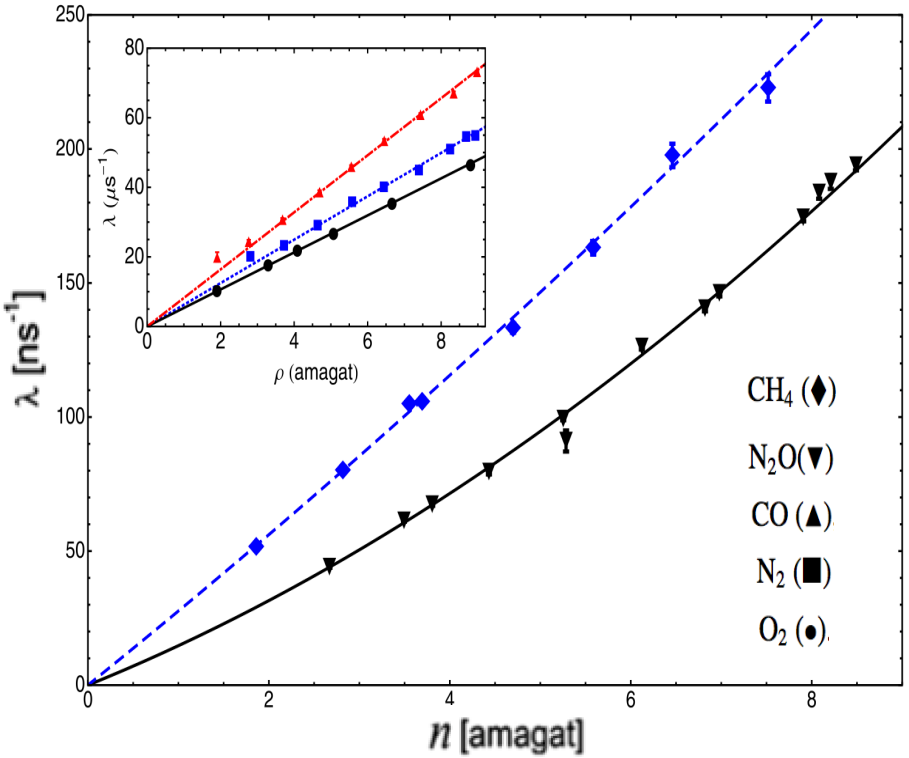
Positron annihilation in condensed matter
(dense gases, liquids, solids)

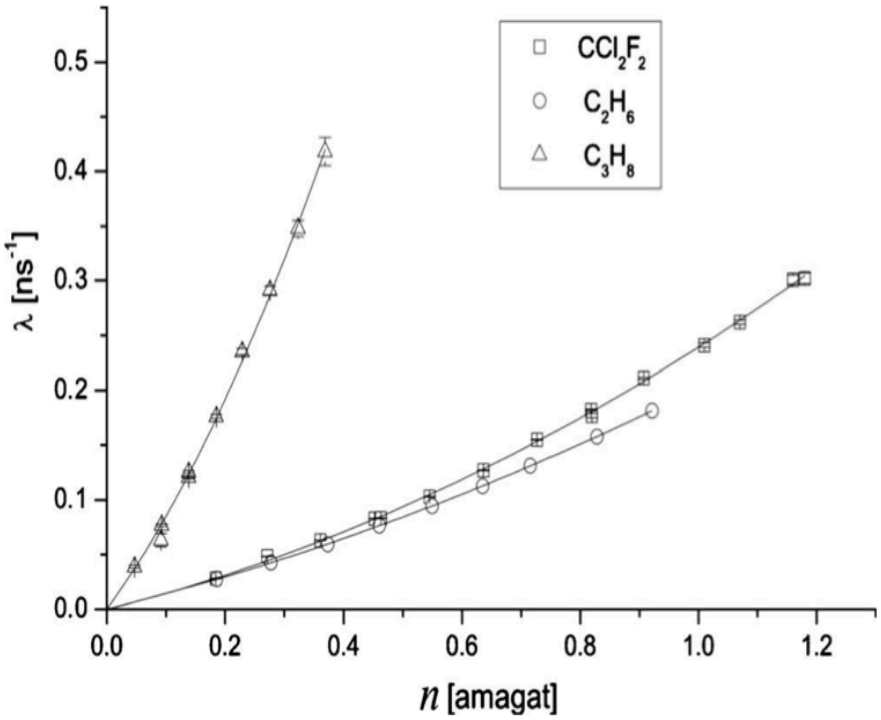


Single positron – atom / molecule interaction is modified by the presence of neighbours.

Annihilation rate as a nonlinear function of gas density

rates of direct e^+ - e^- annihilation derived from PALS measurements





M. Charlton et al.J. Phys. B: At. Mol. Opt. Phys., 46, 195001 (2013)

$$\lambda = \pi r_0^2 c Z_{\text{eff}} n + b n^2$$

Room temperature PALS results for liquid C_6H_6, C_6H_{12} and C_6H_{14}

compared to gas phase experiments

Z_{eff} determined in liquids using a 3-term exponential analysis of lifetime spectra; suposing that an intermediate component (τ_2) corresponds to direct annihilation and *a priori* assuming a linear dependence on liquid density:

$$Z_{\text{eff}} = \left(\pi r_0^2 c n \tau_2\right)^{-1}$$

	liquid phase		gas phase**
Molecule	**present Z_{eff}**	**Mogensen* Z_{eff}**	**$< Z_{eff} >_{th}$**
C_6H_{14} 50 electrons	54	61	120 000
C_6H_{12} 48 electrons	48	51	20 000
C_6H_6 42 electrons	37	45	15 000

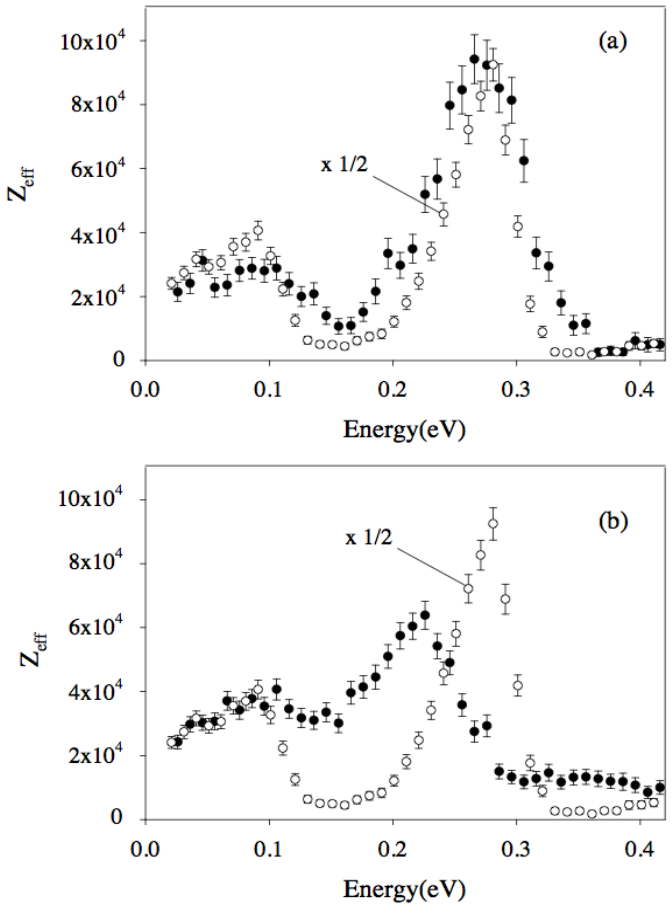


Figure 4.17: The energy-resolved Z_{eff} spectra for (a, •) cyclohexane (C_6H_{12}); and (b, •) benzene (C_6H_6). In both figures, the open circles are the data for hexane (C_6H_{14}) scaled by 0.5 for ease of comparison.

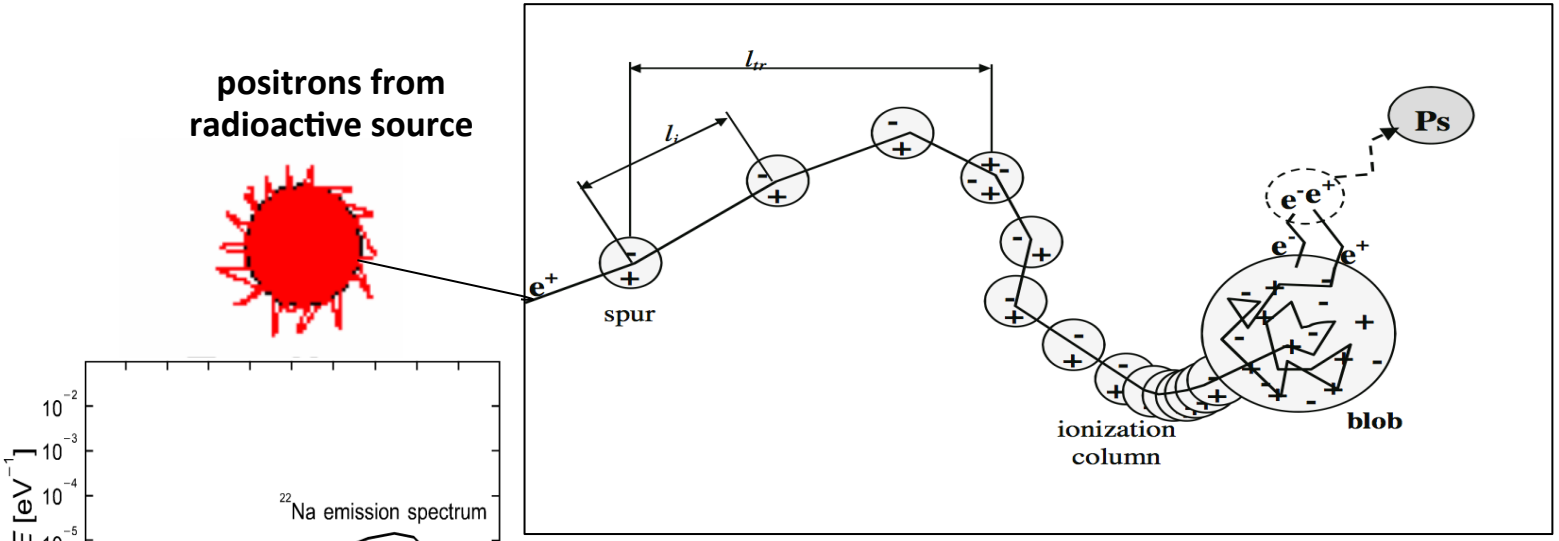
*O. E. Mogensen, „Positron Annihilation in Chemistry", Springer-Verlag, Berlin 1995.

** K. Iwata, R. G. Greaves, and C. M. Surko
"Gamma-ray spectra from positron annihilation on atoms and molecules"
Phys. Rev. A 55 (1997), pp. 3586-3604.

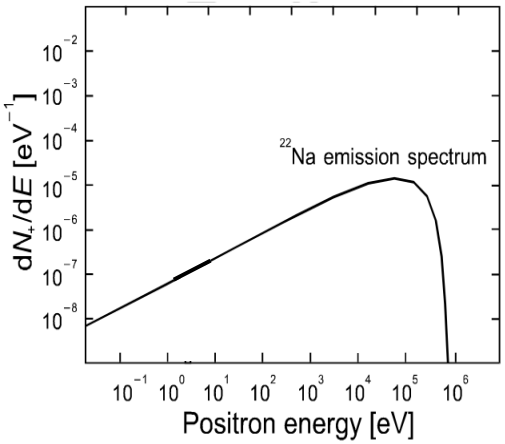
L. D. Barnes
Positron annihilation on atoms and molecules, Ph.D. thesis, University of California, San Diego, 2005 (unpublished).

Energy-resolved annihilation spectroscopy in gas and condensed media at very low positron energies?

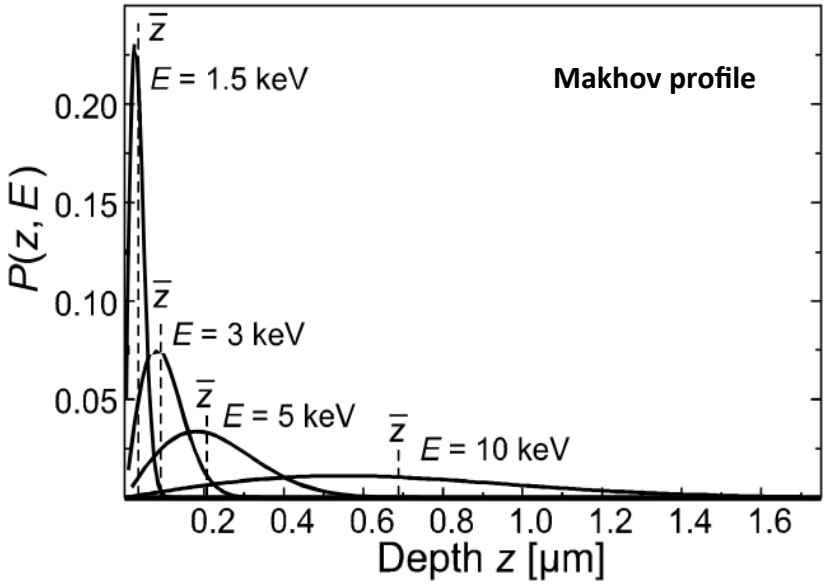
positrons from radioactive source



T. Goworek., Annales UMCS, Section AA – Chemia, vol. LXIX, (2015)



O. E. Mogensen, „Positron Annihilation in Chemistry", Springer-Verlag, Berlin 1995.



Single-particle positron potentials

PHYSICAL REVIEW A **89**, 052707 (2014)

Full-correlation single-particle positron potentials for a positron and positronium interacting with atoms

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(Received 8 March 2014; published 13 May 2014)

In this work, we define single-particle potentials for a positron and a positronium atom interacting with light atoms (H, He, Li, and Be) by inverting a single-particle Schrödinger equation. For this purpose, we use accurate energies and positron densities obtained from the many-body wave function of the corresponding positronic systems. The introduced potentials describe the exact correlations for the calculated systems including the formation of a positronium atom. We show that the scattering lengths and the low-energy *s*-wave phase shifts from accurate many-body calculations are well accounted for by the introduced potential. We also calculate self-consistent two-component density-functional-theory positron potentials and densities for the bound positronic systems within the local-density approximation. They are in a very good agreement with the many-body results, provided that the finite-positron-density electron-positron correlation potential is used, and they can also describe systems comprising a positronium atom. We argue that the introduced single-particle positron potentials defined for single molecules are transferable to the condensed phase when the intermolecular interactions are weak. When this condition is fulfilled, the total positron potential can be constructed in a good approximation as the superposition of the molecular potentials.

THE JOURNAL OF PHYSICAL CHEMISTRY B

Article

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Pick-Off Annihilation of Positronium in Matter Using Full Correlation Single Particle Potentials: Solid He

A. Zubiaga,*[,†] F. Tuomisto,[†] and M. J. Puska[‡]

DOI: 10.1021/jp5106295
J. Phys. Chem. B 2015, 119, 1747−1755

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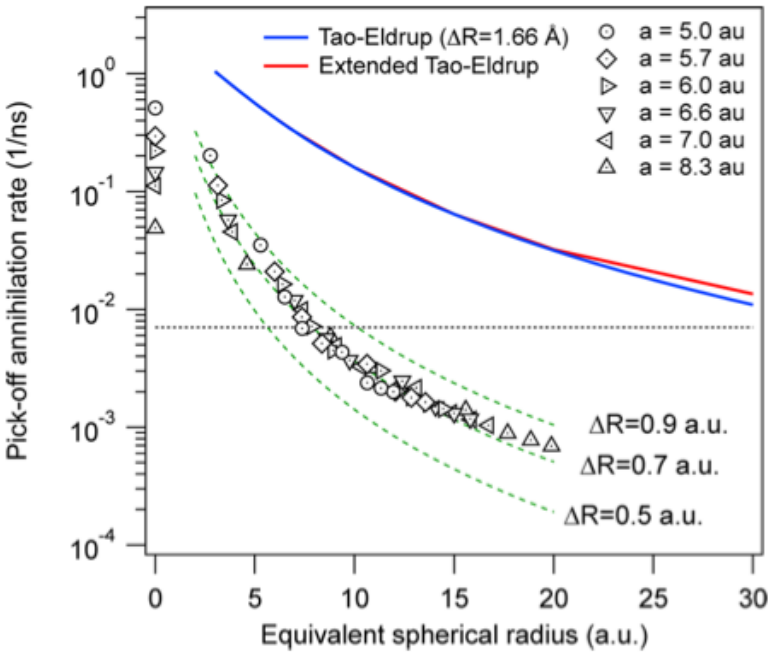

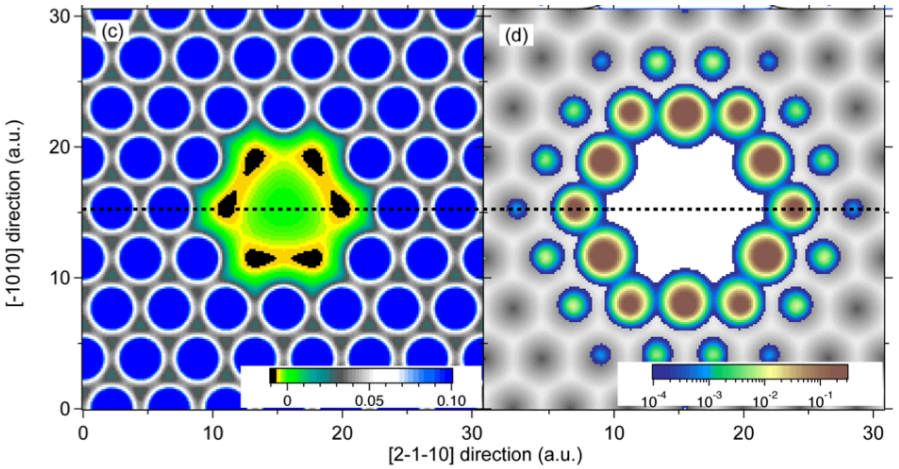

$$\lambda_{\mathrm{TE}}^{\mathrm{po}} = 2.0\ (\mathrm{ns}^{-1})\left[1 - \frac{R}{R+\Delta R} + \frac{1}{2\pi}\sin\left(\frac{2\pi R}{R+\Delta R}\right)\right]$$

Thank you for your attention