List of Slides

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TSAPS Fall 2003

Results for Positron-Acetylene Scattering Using the Distributed Positron Model

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Special thanks to **Mr. Lee Burnside** for cluster construction and maintenance.

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Abstract for TSAPS 2003

Results for Positron-Acetylene Scattering Using the Distributed Positron Model, THOMAS L. GIBSON, Texas Tech University, and PATRICK J. NICHOLS, University of New Orleans — The Distributed Positron Model (DPM) has been developed as a means to include the correlation/polarization interaction between a slow positron and an atomic or molecular target. This technique is based on a quantum chemistry approach that approximates the effect of virtual positronium formation near the target and automatically reduces to the correct long-range form of the polarization potential far from the target. Further, the codes that implement our DPM method have been written to run on low-cost concurrent computers known as GNU/Linux Beowulf clusters. In this talk we will report integrated and differential cross sections for low-energy positron-acetylene collisions.

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Motivation

Why calculate low-energy positron-molecule collisions?

- Very few measured results available
  - Intense low-energy beams are hard to acheive
- Existing experiments don't agree
- Most theories too parameterized or intractable for larger systems

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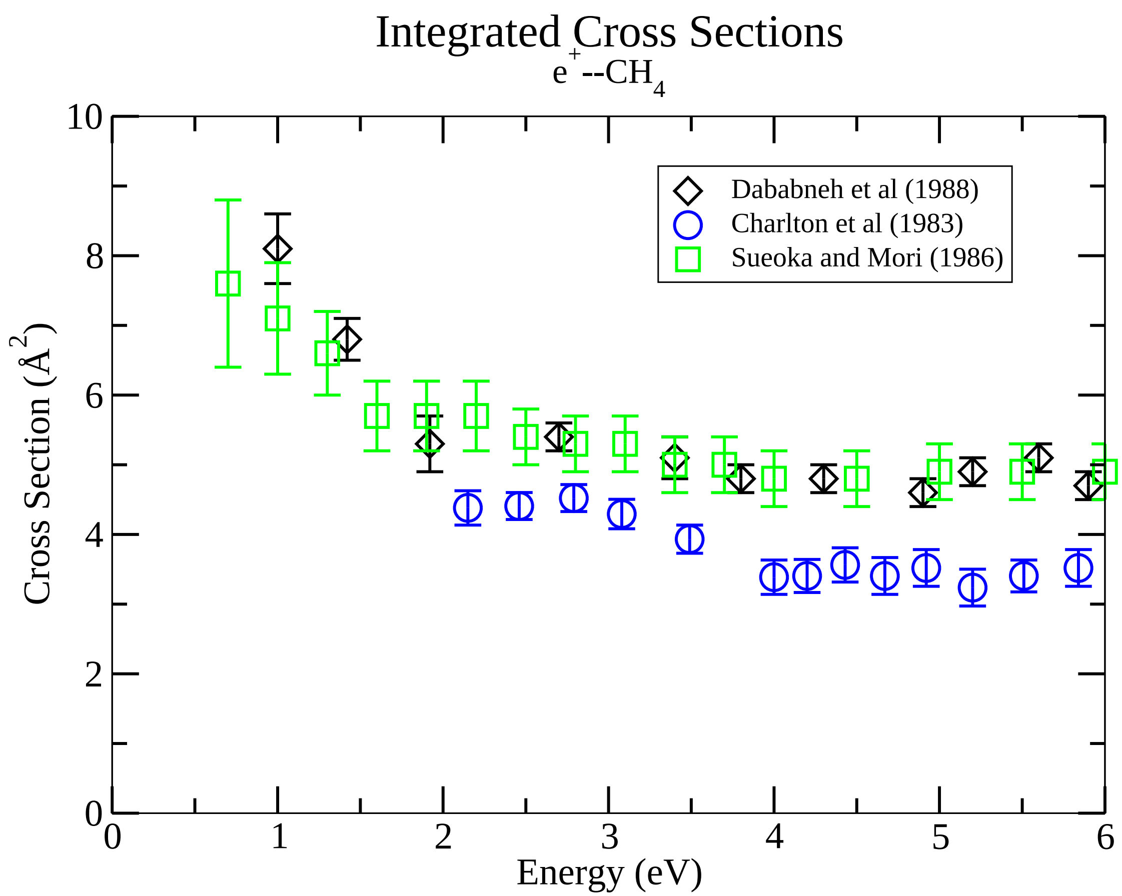
Positron-CH_4



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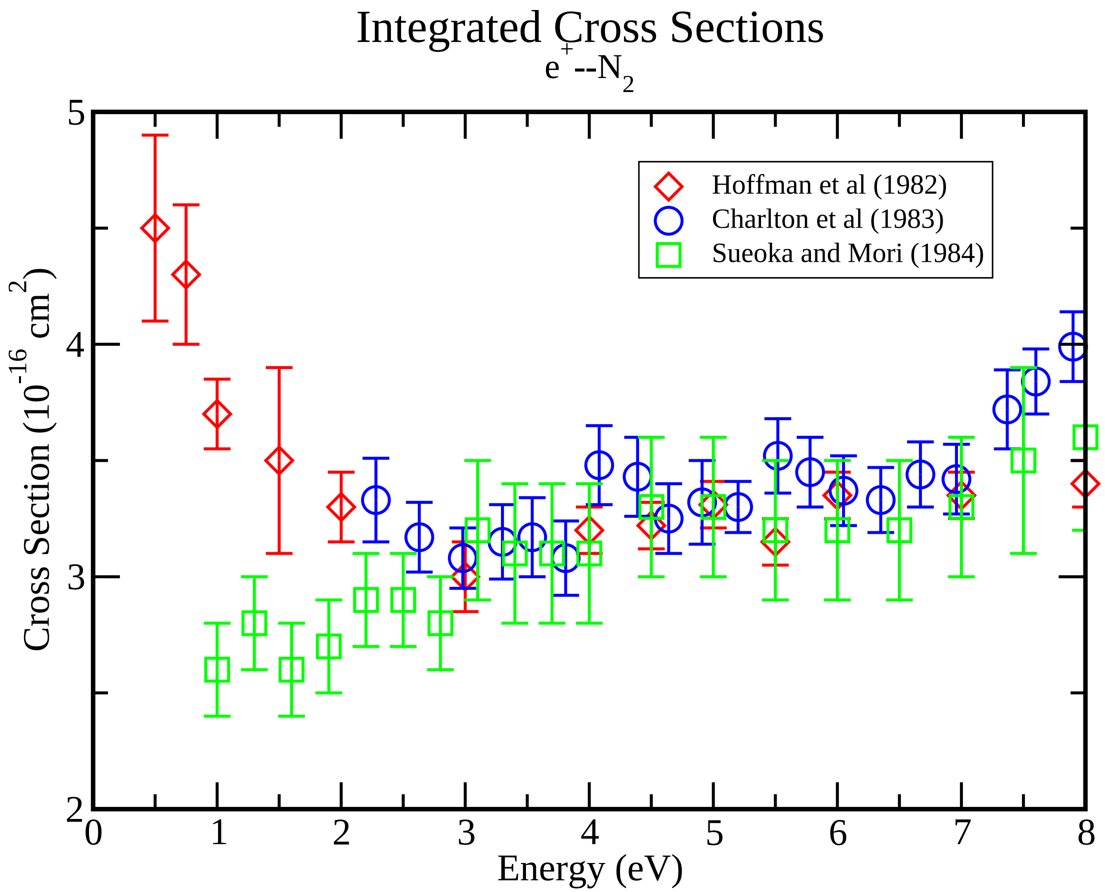
Positron-N_2



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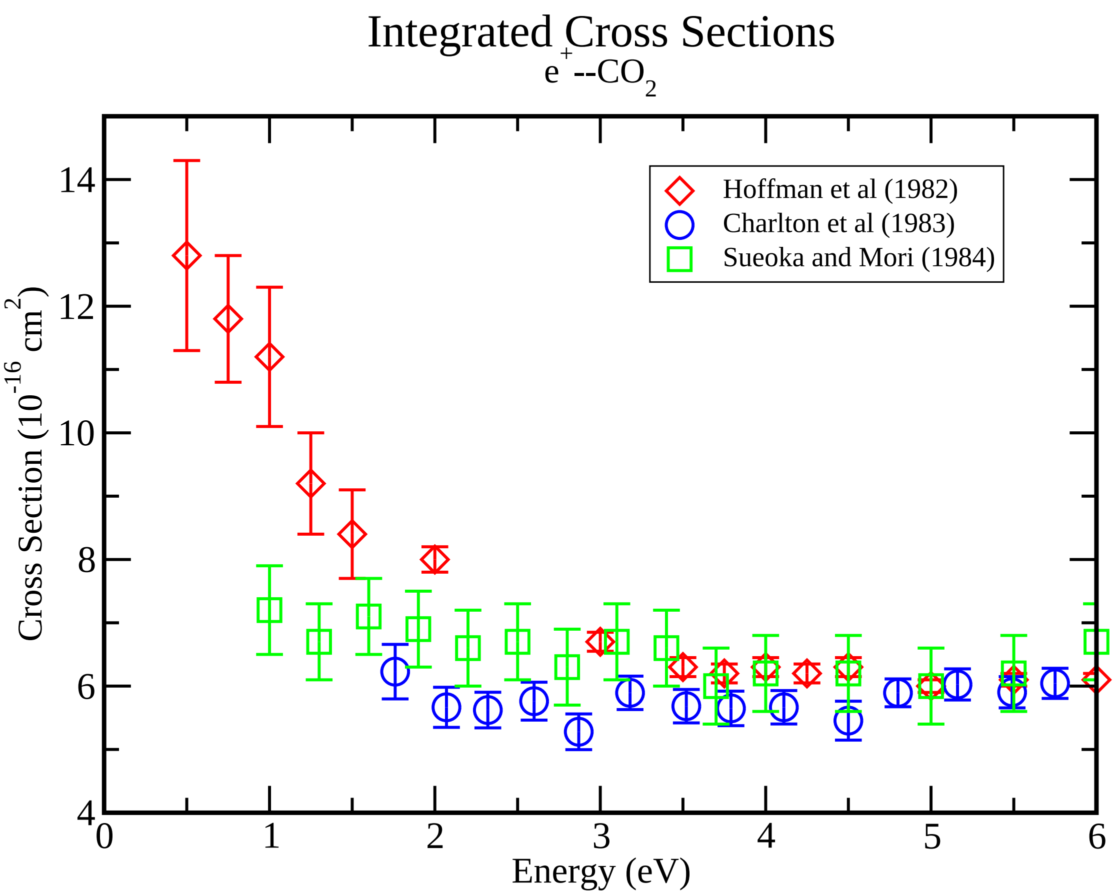
Positron-CO_2



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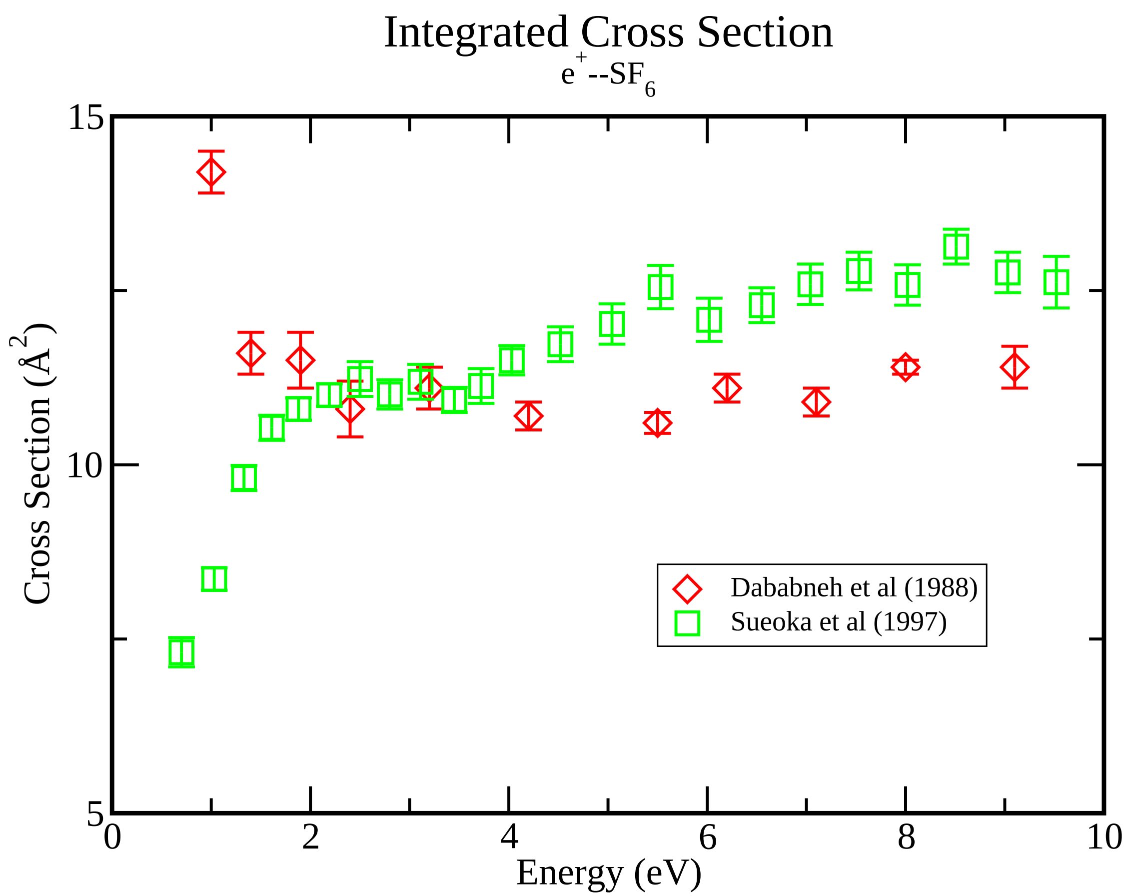
Positron-SF_6



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Our Theoretical Treatment

- Isolated collision between one target (atom or molecule) and one positron of known kinetic energy
- Only elastic scattering—stay below the energy threshold for electronic excitation of the target or for real positronium formation
- Local, energy-independent interaction potential based on physically-motivated approximations

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Reduction of Scattering Formulation

We "reduce" the problem by expanding the (N+1)-particle ket in a complete set of target and scattering states, viz.

$$|\Psi> = \sum\!\!\!\!\!\!\int_\gamma F_\gamma \Phi_\gamma .$$

Using this expansion in the T.I.S.E. and operating on the left with $< \Phi_0|$ eventually leaves the one-particle T.I.S.E. for elastic scattering of the positron

$$\hat{T}_p|F_0 > \, - \frac{k^2}{2}|F_0 > = -\hat{V}_{sp}|F_0 > .$$

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Interaction Potential

A local approximation to the interaction potential between a colliding positron and the molecular target can be represented as

$$V_{sp}(\vec{r}_p) \;=\; V_{st}(\vec{r}_p) \;+\; V_{pol}(\vec{r}_p),$$

where the static potential is given by,

$$V_{st}(\vec{r}_p) \;=\; \left\langle \Phi_0(\vec{r}_i) \left| \hat{V}_{int} \right| \Phi_0(\vec{r}_i) \right\rangle,$$

with $\hat{V}_{int}$ representing the Coulomb interactions between the positron and the target and where $V_{pol}(\vec{r}_p)$ is the polarization potential.

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Polarization Potential

The polarization potential is defined as the energy difference

$$V_{pol}(\vec{r}_p) \;=\; E^R(\vec{r}_p) - E^U(\vec{r}_p),$$

where the energy from the relaxed (distorted) target orbitals is

$$E^R(\vec{r}_p) \;=\; \left\langle \Phi^R(\vec{r}_i;\vec{r}_p) \left| \hat{\mathcal{H}}_t + \hat{V}_{int} \right| \Phi^R(\vec{r}_i;\vec{r}_p) \right\rangle_{d\vec{r}_i},$$

and the energy from the unrelaxed (ground state) orbitals is

$$E^U(\vec{r}_p) \;=\; \left\langle \Phi_0^U(\vec{r}_i) \left| \hat{\mathcal{H}}_t + \hat{V}_{int} \right| \Phi_0^U(\vec{r}_i) \right\rangle_{d\vec{r}_i}.$$

In the adiabatic approximation, both $E^U(\vec{r}_p)$ and $E^R(\vec{r}_p)$ are calculated by treating the projectile as an additional "proton" (located at $\vec{r}_p$) and using an LCAO:MO—SCF Quantum Chemistry code to provide variational estimates of these energies.

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Nuclear Attraction Integrals

The distortion of the molecular orbitals is driven by the nuclear attraction integrals that involve the positron as an additional "nucleus" at $\vec{r}_p$.

$$I_{i,j}^{NAI} = \langle \alpha_i(\vec{r}_e) \, | V(\vec{r}_e; \rho_{pos}) | \, \beta_j(\vec{r}_e) \rangle \, ,$$

where the interaction V from a distribution of positive charge ρ_{pos} is given as

$$V(\vec{r}_e; \rho_{pos}) = \int d\vec{r} \, \rho_{pos}(\vec{r}) \, \frac{-1}{|\vec{r}_e - \vec{r}|} .$$

For the adiabatic approximation, $\rho_{pos}(\vec{r}) = \delta(\vec{r} - \vec{r}_p)$, which is appropriate for the positive charge distribution in a virtual H atom.

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Virtual Positronium vs Virtual Hydrogen

- Adiabatic approximation is much too attractive in the near-target region
- Use ρ_{pos} more nearly correct for virtual Ps
  - Hence, the name Distributed Positron Approximation (DPM)

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Ps C.O.M. Figure

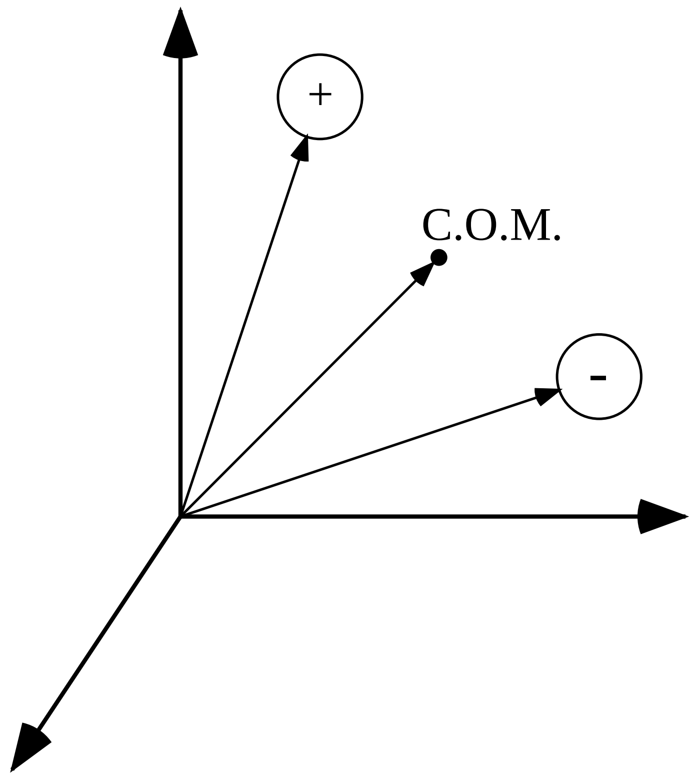

Figure 1: Unlike the H atom, the positive charge in the Ps atom is not localized at the C.O.M. of the atom.

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The Distributed Positron Model

We have investigated several simple choices of ρ_{pos} that reflect the distribution of positive charge in a Ps atom and lead to a polarization potential that reduces to the correct long-range behavior of the polarization potential, including:

- Uniform Spherical
  - $R_p = 1.5$ Bohr (Average radius of Ps atom)
  - $R_p = 1.0$ Bohr (Maximum radial probability of Ps atom)
- H1S distribution
- STO-3G distribution

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DPM Figure

For specificity, consider the following case:

- Diatomic target with nuclei at $\vec{A}$ and $\vec{B}$
- Additional "nucleus" (positron) with charge distribution ρ_{pos} located at $\vec{C} \equiv \vec{r}_p$

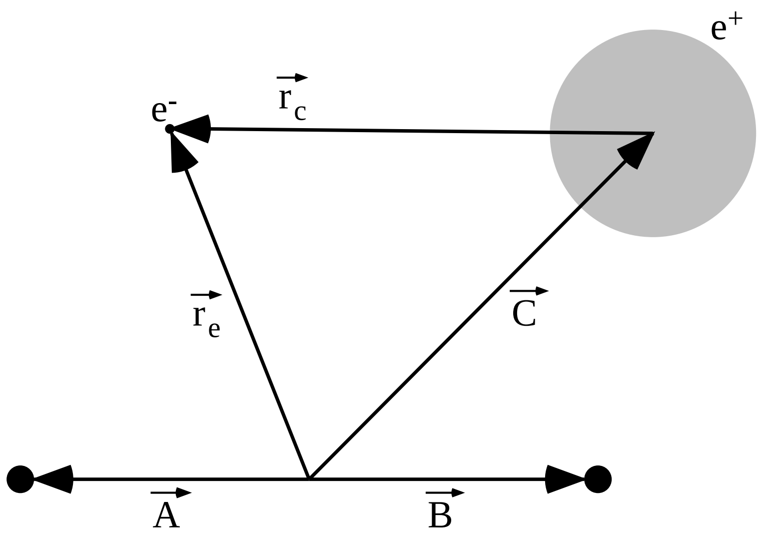

Figure 2: A distribution of positive charge simulates the effect of virtual Ps formation in the DPM.

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DPM Distortion Interaction Figure

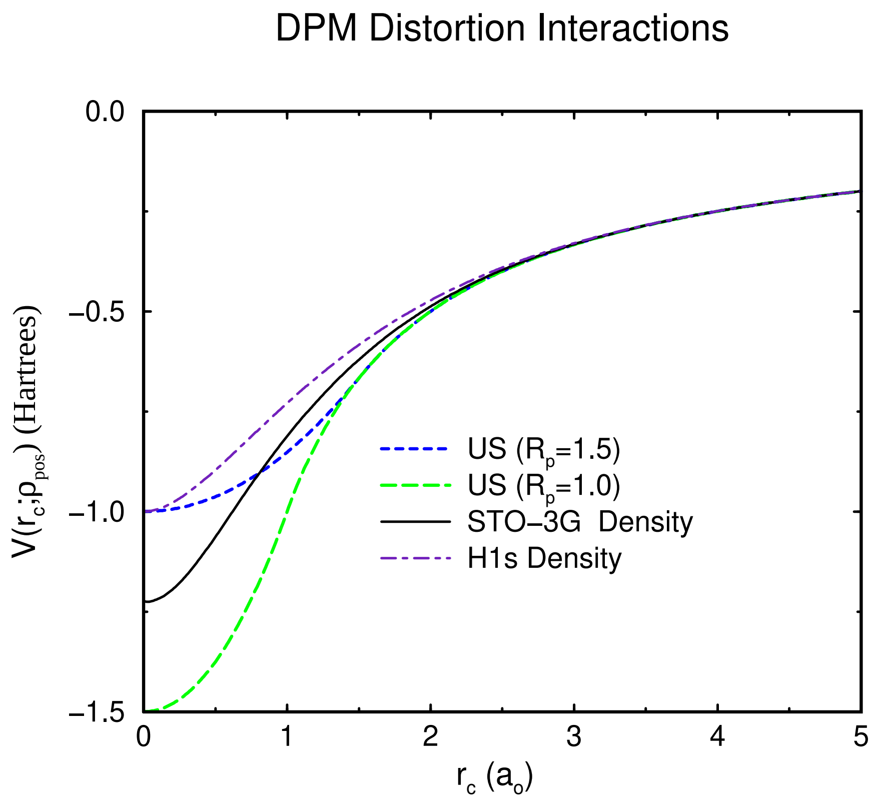

Figure 3: The distortion interaction $V(\vec{r}_c;\rho_{pos})$ for various choices of ρ_{pos} in the DPM.

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Computing the Interaction Potential

To calculate the polarization component of the interaction potential, we fix the positron at a large number of points near the target and then compute a variational estimate of the system energy for each of these points.

- **Bigger Systems $\Longrightarrow$ More CPU Time**
  - Time to compute V_{pol} for Ar: 12 minutes (serial code)
  - Time to compute V_{pol} for SF_6: 125 days (estimated)
- **Bigger Systems $\Longrightarrow$ More Memory**
- **Bigger Systems $\Longrightarrow$ More I/O**

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Solution

- **Beowulf Cluster**
  - Performance: 100's to 1000's of Megaflops
  - Memory: Gigabytes
  - I/O: Distributed Across Multiple Nodes
  - **Very** Affordable Hardware
  - Standard Software Available for Free
  - Local Control
    * Configuration Optimized for Problem
    * No Sharing Required

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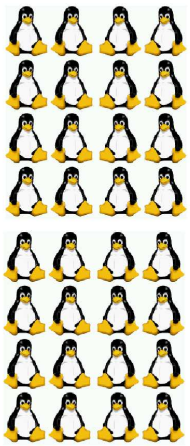
Gamera Mark II



$\Rightarrow$

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Gamera Mark II Hardware

- 32 1-GHz Athlon CPUs
- 16 Gigabytes aggregate ram
- 640 Gigabytes aggregate disk
- 2 100 base-T 24-port switches
- **Cost** $\sim$ \$30,000

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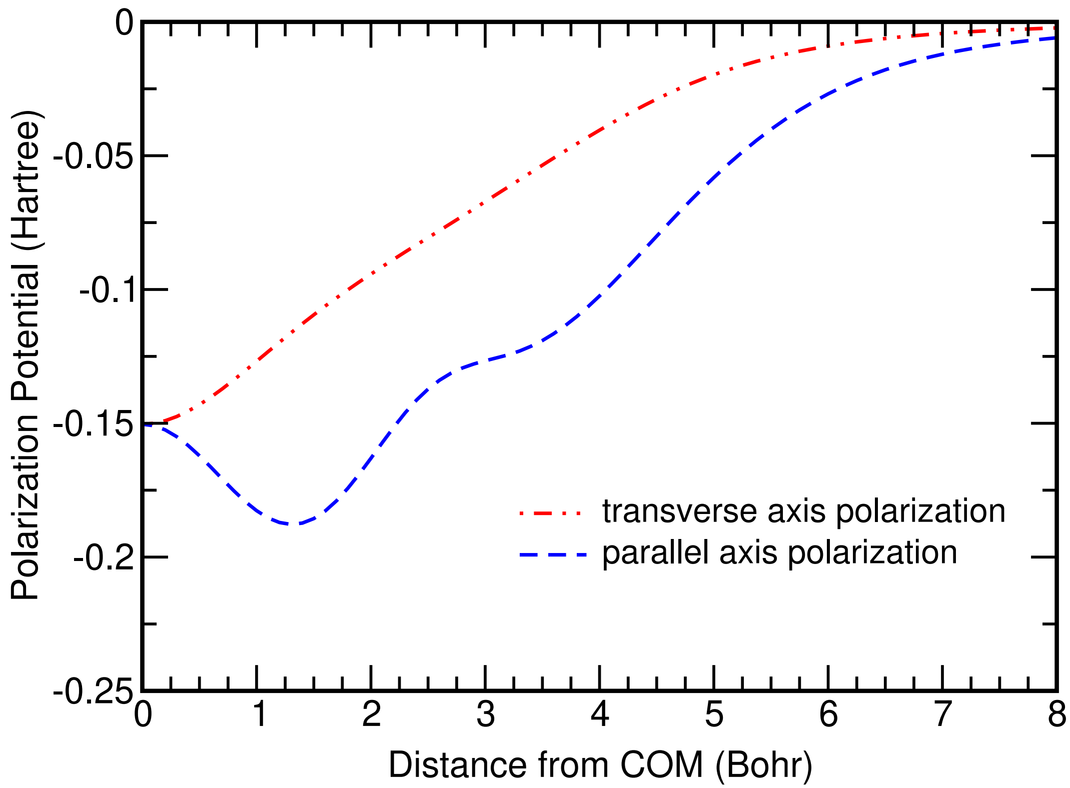
Positron-C_2H_2 Polarization Potential



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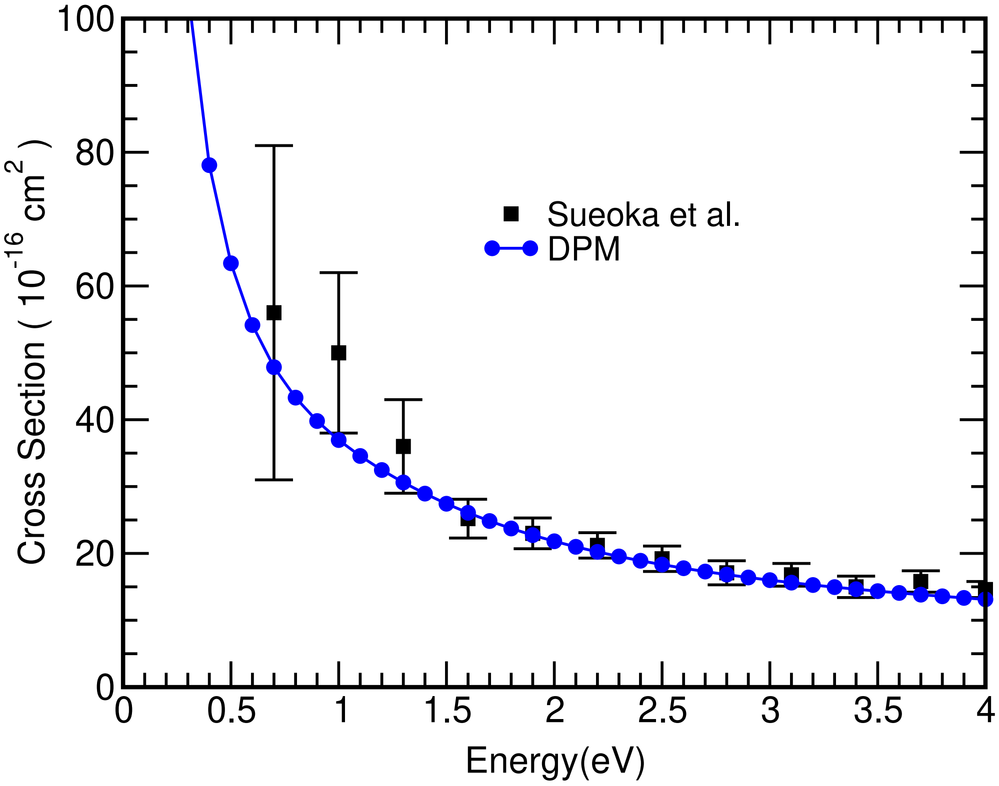
Positron-C_2H_2 Integrated Cross Sections



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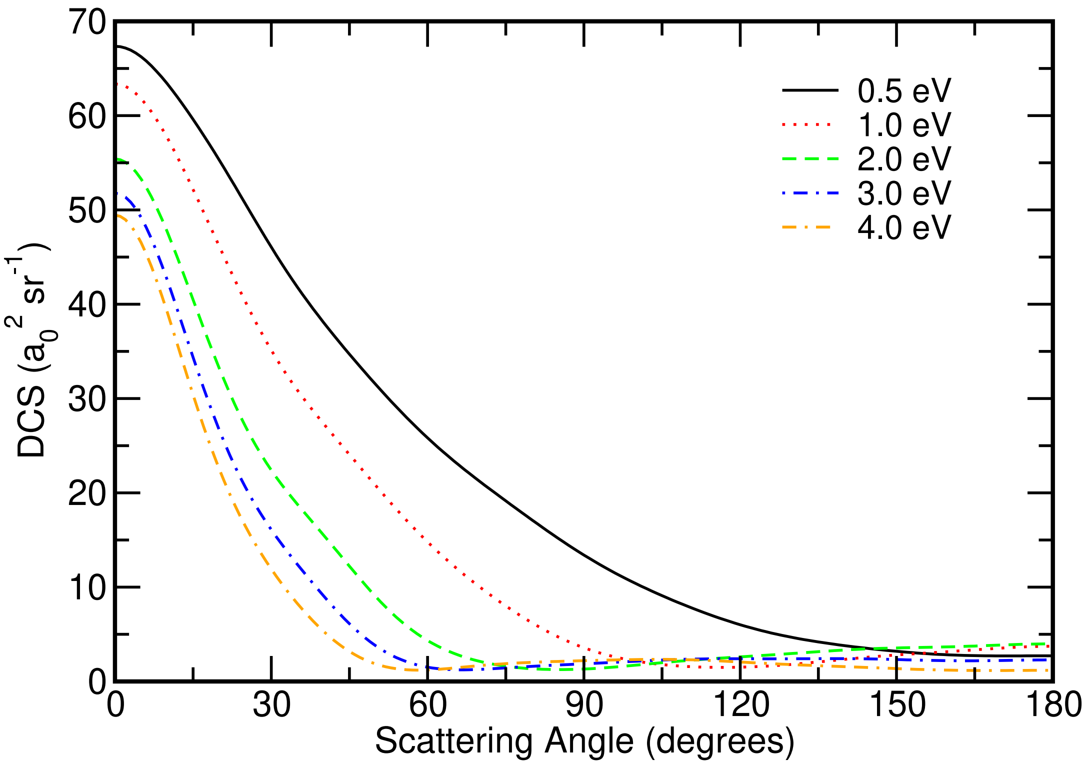
Positron-C_2H_2 Differential Cross Sections



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Conclusions

- High-Performance Computing $\equiv$ Concurrent Computing
- Affordable Parallel Systems Are Available Now
- Open Source Software and Scientific Applications Are Compatible
- The DPM has been shown to yield consistently good agreement with measured low-energy positron-atom and positron-molecule collisions

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We are grateful for the collaborative efforts of Dr. Robert Lucchese and Dr. Franco Gianturco on the CH_4 and SF_6 systems, as well as our continuing work on C_8H_8.

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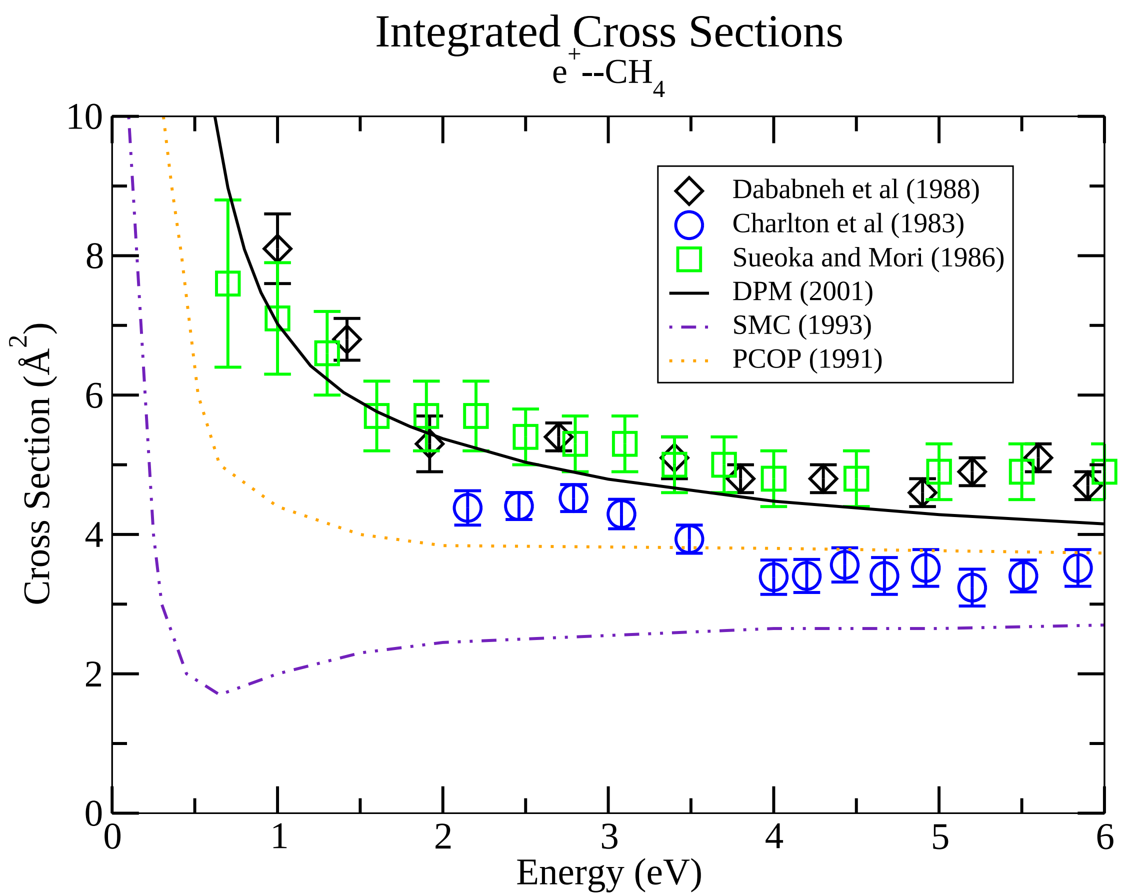
Positron-CH_4 Cross Sections



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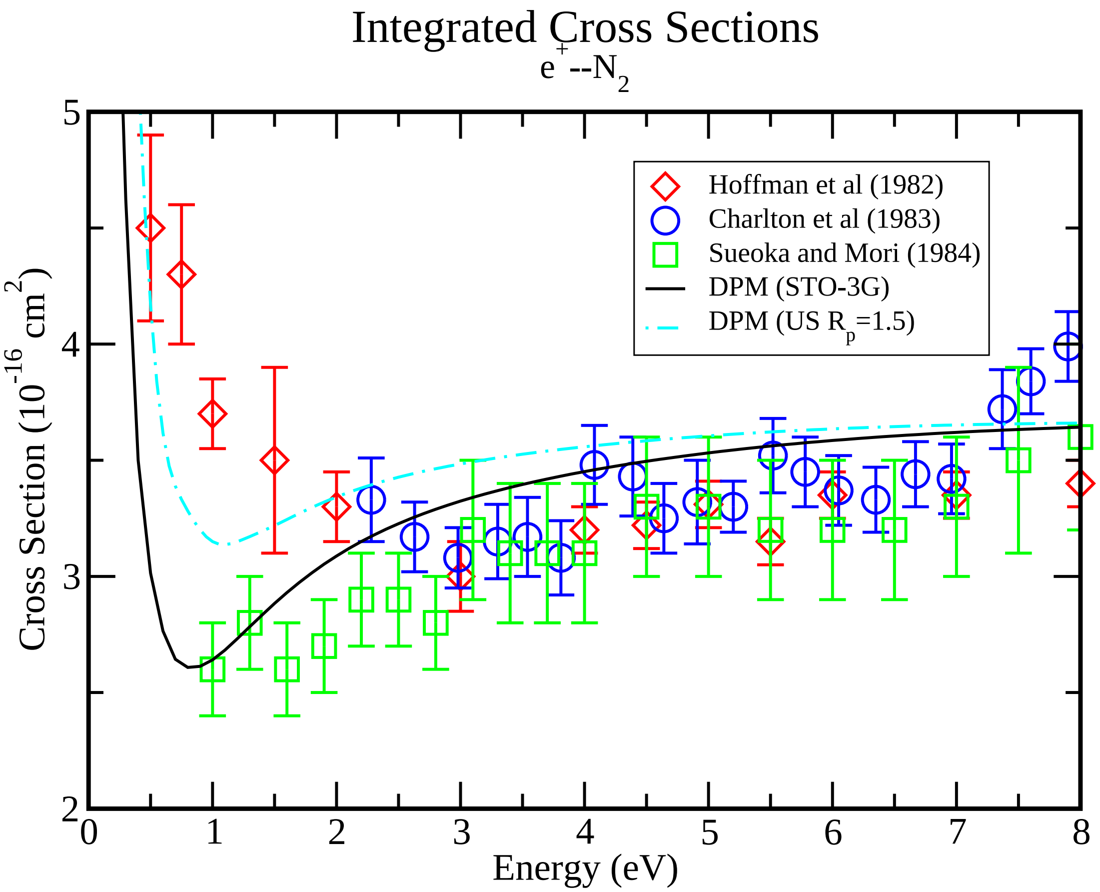
Positron-N_2 Cross Sections



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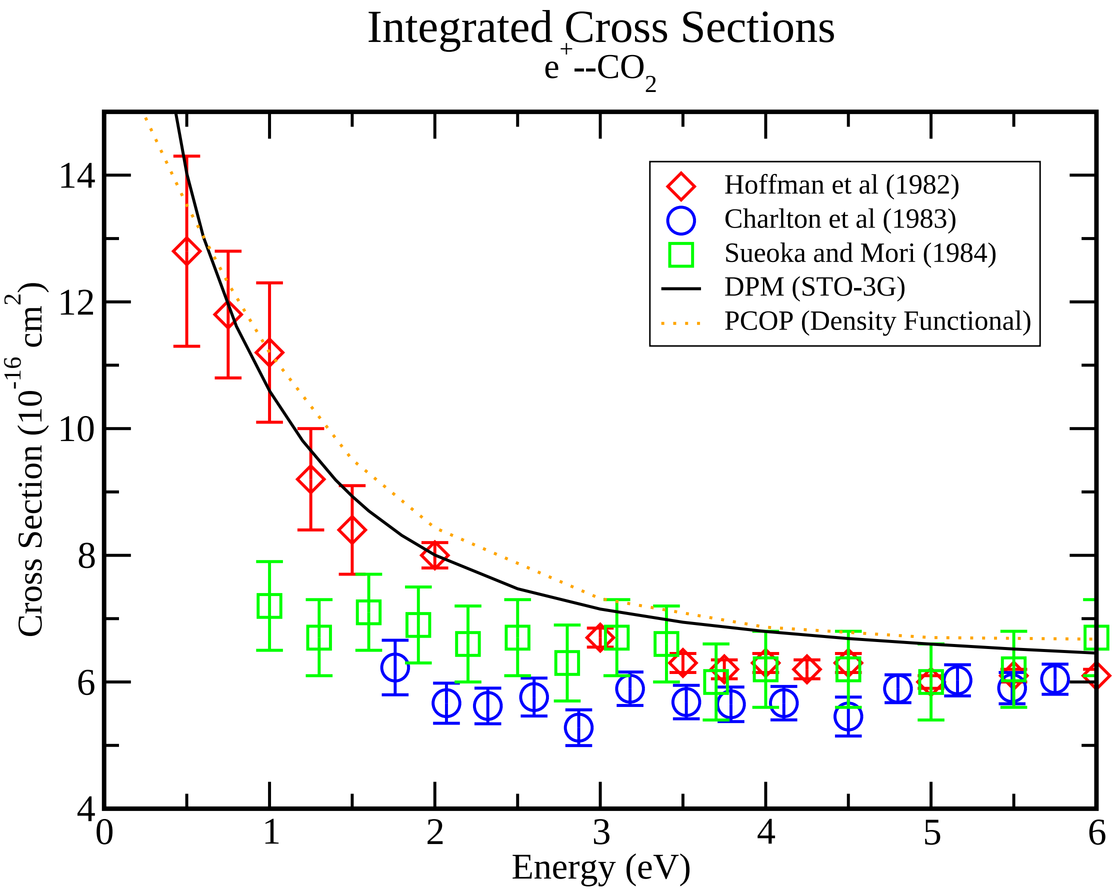
Positron-CO_2 Cross Sections



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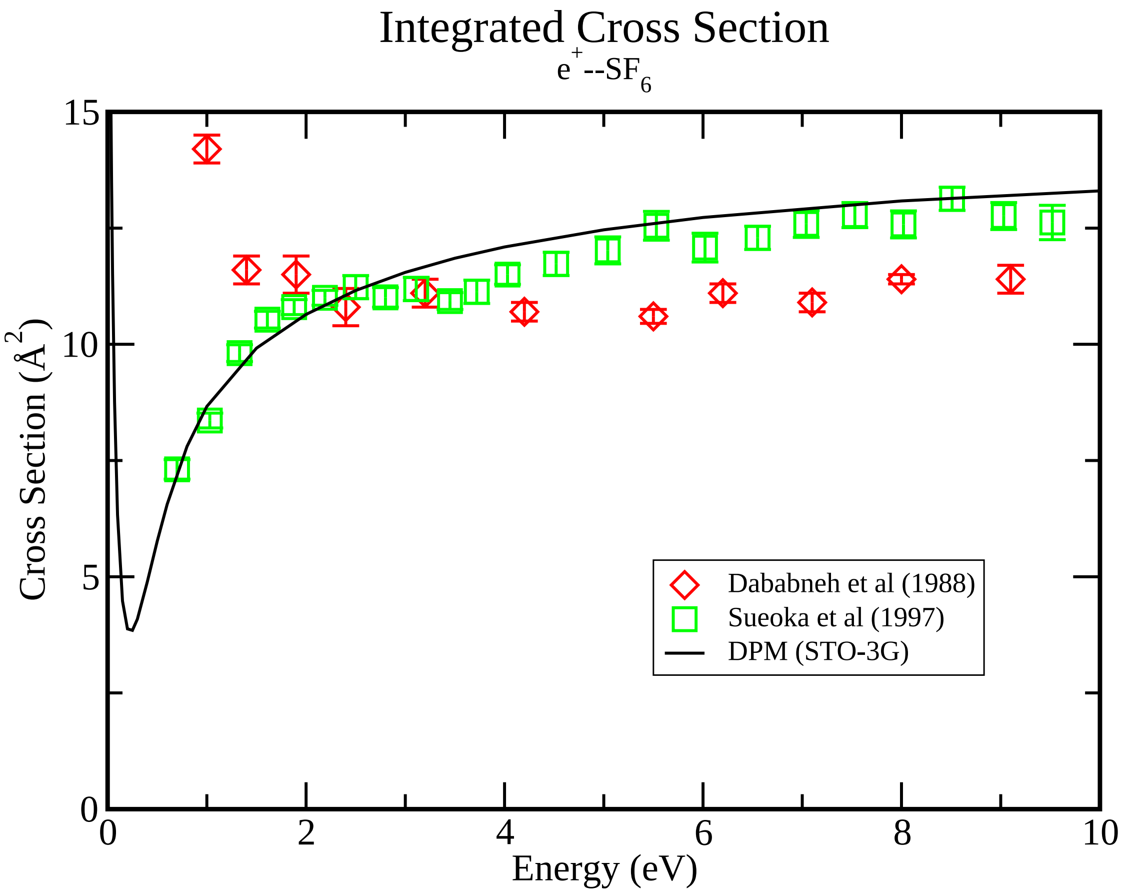
Positron-SF_6 Cross Sections - Close



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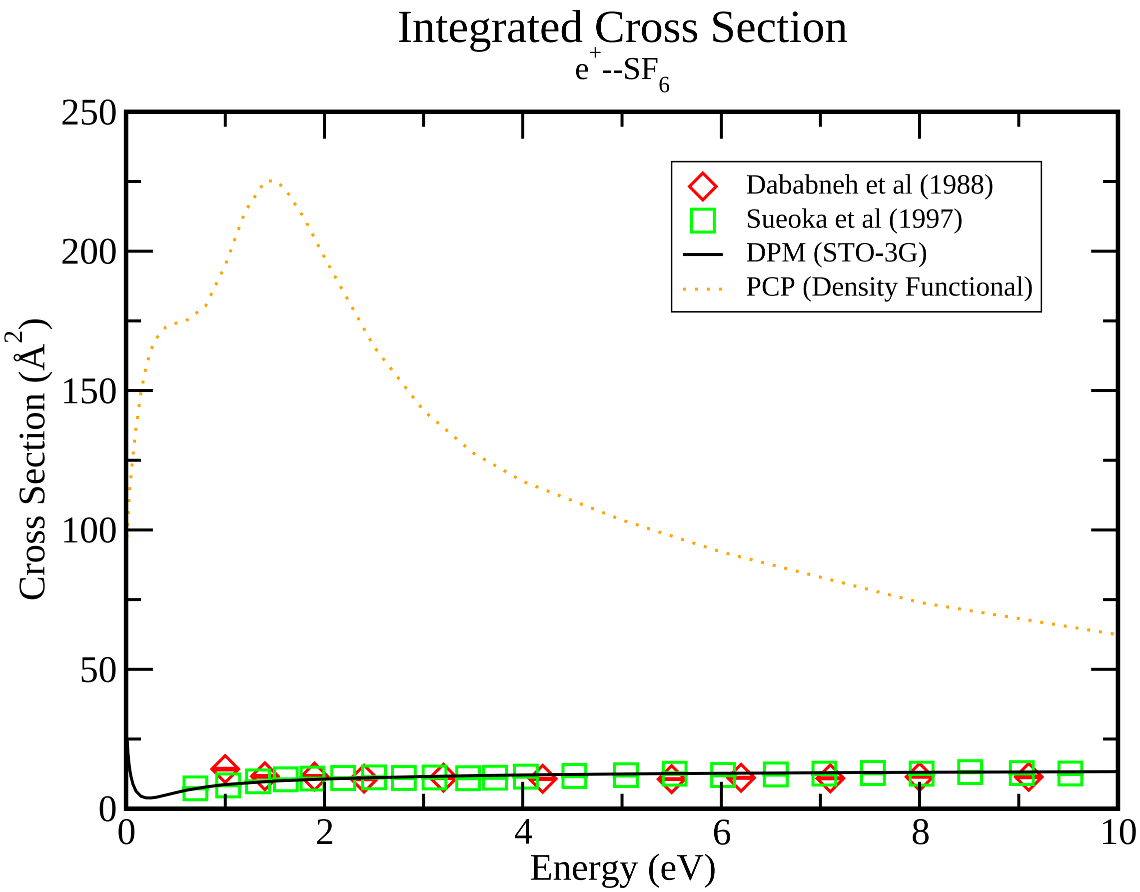
Positron-SF_6 Cross Sections - Far



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C_2H_2 Properties - 1

Table 1: Total Energies

Research Group	**Energy** (Hartree)
this work	-76.84885
Jameson and Fowler	-76.84857
Lindh and Liu	-76.85500

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C_2H_2 Properties - 2

Table 2: Quadrupole Moments

Group	θ(au)
this work	5.43
Jameson and Fowler	5.47
Amos	5.47
Lindh and Liu	5.24-5.44
experimental	2.23-6.24

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C_2H_2 Properties - 3

Table 3: Polarizabilities

Research Group	$\overline{\alpha}$	α_{zz}	α_{xx}
this work	21.22	32.95	15.35
Jameson and Fowler	23.11	31.34	19.34
Gough	22.68		
Gough	14.30	24.842	9.025
experimental	23.53	31.91	19.34

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