

Elastic positron scattering from H₂, N₂ e O₂ using ab initio potentials.

Denise Assafrão¹, Kaio Mazon², Luis Poveda³ e J. R. Mohallem⁴

¹Departamento de Física, Centro de Ciências Exatas, Universidade Federal do Espírito Santo, Vitória, ES, Brasil.

²Departamento de Física, Centro de Ciências Físicas e Matemática, Universidade Federal de Santa Catarina, Florianópolis, SC, Brasil.

³ Departamento de Física e Matemática , Centro Federal de Educação Tecnológica de Minas Gerais, Belo Horizonte, MG, Brasil.

⁴Laboratório de Átomos e Moléculas Especiais, Departamento de Física, ICEx, Universidade Federal de Minas Gerais, Belo Horizonte, MG, Brasil.

denise.lima@ufes.br, rachid@fisica.ufmg.br

Positron scattering by molecules, even the simplest ones, is a difficult theoretical many- body problem, so that few applications aiming at the calculation of scattering cross sections can be found in the literature. In this work we develop semi empirical local potentials for positron scattering from diatomic molecules. Since the positron is treated on the same footing of the nuclei here[1], the problem becomes to produce a PES for three-center systems. We obtained a set of ab initio points and applied this methodology for positron scattering from H₂, N₂ e O₂. The ad hoc inclusion of a long range polarization term is needed only for H₂, which gives our calculations an ab initio character. Scattering cross sections are obtained with a MCF [2] routine [3]. Our results is compared to different theoretical and experimental results with very good agreement.

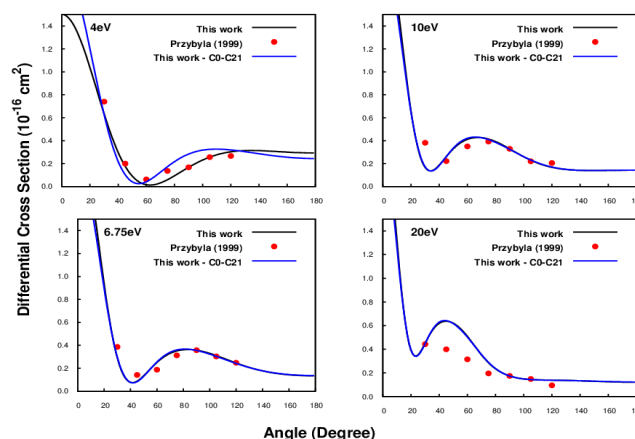


Figure 1: Differential Cross Section for positron scattering from O₂ using the ab initio local potential.

References

- [1] Luis A Poveda, Adriano Dutra, J. R. Mohallem, and Denise Assafrão, Physical Review. A, **87**,(2013), 052702.
- [2] J. Horáček and T. Sasakawa, Phys. Rev. A. **28** (1983), 2151.
- [3] M.-T. Lee and I. Iga, J. Phys. B, **32** (1999), 453.

Acknowledgement: **FAPES. FAPEMIG, CNPq**