Low energy positron scattering from Cl_2 using a model potential to describe polarization in positron-molecule scattering.

Sidnei G. Fabris Jr*, Francisco F. Frighetto, Alessandra Souza Barbosa, Sergio D'A. Sanchez

[1] *Departamento de Física, Universidade Federal do Paraná, Curitiba - PR, Brasil*

*e-mail: sidneifabris@ufpr.br

There has been an increasing interest in positron physics due to its technological and biological applications as well as its importance in fundamental physics. In particular, the positron interaction with atoms and molecules is a cornerstone of this knowledge, since many applications are based on basic interactions with molecules and atoms. For instance, positron annihilation is a core concept in the positron emission tomography (PET) scan for diagnostics in medicine [1].

The cross sections were obtained with Schwinger multichannel method (SMC) implemented for positron scattering [2] and incorporated the computational detail using basis functions and adding extra functions centered to better capture the polarization potential, using the same framework as Frighetto, Barbosa and Sanchez [3].

Here, we will present calculated cross section for positron collisions with chlorine gas obtained with the most recent parallelized version of the Schwinger Multichannel Method for positron scattering [3] that allows us better time-performance in our calculations. We have also carried out additional calculations employing the model potential proposed by Swann and Gribakin [4-6] and already implemented in our codes [3].

By comparing calculations, we were able to obtain the free parameter of the model potential for the chlorine atom which better describes our fully ab-initio calculation for Cl_2. In further works, we intend to use the same value of ρ to obtain data for bigger systems such as $C_2H_2Cl_2$ and C_2Cl_2

References

1. S. I. Ziegler, Positron emission tomography: Principles, technology, and recent developments, Nucl. Phys. A 752, 679 (2005).
2. J.S.E.Germano and M.A.P.Lima, Phys.Rev. A47,3976(1993).
3. F. F. Frighetto, A. Souza Barbosa and S. d'A. Sanchez, Implementation of a model potential in the Schwinger multichannel method to describe polarization in positron-atom and -molecule scattering: Studies for the noble-gas atoms, H2, and N2, Phys. Rev A 108, 012818 (2023)
4. A. R. Swann and G. F. Gribakin, Calculations of positron binding, and annihilation in polyatomic molecules, J. Chem. Phys. 149, 244305 (2018).
5. A. R. Swann and G. F. Gribakin, Phys. Rev. A 101, 022702 (2020).
6. A. R. Swann, G. F. Gribakin, J. R. Danielson, S. Ghosh, M. R. Natisin, and C. M. Surko, Phys. Rev. A 104, 012813 (2021).