Positronium Annihilation Spectroscopy: A tool for the study of transport properties of self-assembled lipid biostructures

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The positron annihilation spectroscopy is well suited for the study of the size and density of nanometre scale voids in polymers [1] and molecular materials, including biostructures [2]. Relevant information about the free volume in biostructures, not measurable by other methods, can be obtained. Specially relevant is the information obtained from the pick-off annihilation of orto-Positronium (o-Ps), the S=1 state of a positron and a electron bound state. Its lifetime has been correlated with the rheological properties of lyotropic liquid crystalline phases of self-assembled lipid biostructures [3] and the transition between the gel-fluid phases has been observed [2]. These results will yield to a deeper understanding of the diffusion transport across the membrane of the cells. Experimental results are analyzed using a simple model developed by Tao and Eldrup that predicts a relationship between the Ps lifetime and the pore/void radius [4]. This model has been tested in organic liquids and is able to predict the pore/void radius, but it is only useful in materials with compact pores and it does not take into account the chemical effects due to the variation of the Ps interaction at different host materials.

Ps interaction in molecular materials is similar to other molecules: at large distances it feels an attractive force due to the dispersion interaction with the neutral molecules and at short distances it is repelled due to, mainly, the exchange-correlation interaction between the electrons in the molecule and the Ps [5]. On the other side, the wavefunction of both constituents, the electron and the positron, is always widely widespread inside the host material due to mainly the low mass of both (the mass of Ps is almost 2000 times smaller than H_2, the lightest molecule).

For a deeper understanding of the experimental data, theoretical modeling of the Ps distribution and annihilation properties is needed, in a similar way as for positrons in condensed matter [6]. But before the Ps-matter interaction potential needs to be better understood. This work presents the results on atom-Ps interaction using exact diagonalization and stochastic variational optimization method of correlated gaussian [7] basis.

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