

## PHD PROJECT DESCRIPTION

(4000 characters max., including the aims and work plan to be published online)

### Project title: Positron Interactions with Organic Matter

#### 1.1. Project goals

- (a) Investigation of positron thermalization, trapping, positronium formation, and annihilation in selected organic condensed matter.
- (b) Determination of relationships between PALS parameters and microstructural properties of organic materials, especially free volume, disorder, and composition.
- (c) Verification of the applicability and limitations of standard free-volume models, especially the Tao–Eldrup approach.
- (d) Analysis of selected simple organic molecules as models for interpreting positron and positronium interactions in complex organic matter.
- (e) Adaptation and calibration of the fast–fast coincidence PALS setup for organic samples, with relevance to materials science and positronium imaging.

#### 1.2. Outline

Positron annihilation lifetime spectroscopy (PALS) is a nondestructive technique for studying microstructure. In solids, it is used to investigate defects and their influence on material properties [1]. It has also been applied to atoms, molecules, and molecular substances, providing insight into matter–antimatter interactions [1,2]. Recent interest in positron interactions with organic matter has been stimulated by medical applications, especially PET and positronium imaging [5–7].

In organic condensed matter, positron annihilation involves thermalization, trapping in free-volume sites, positronium (Ps) formation, and annihilation. The lifetime of ortho-positronium (o-Ps) is highly sensitive to the size and distribution of free-volume holes. Therefore, PALS is suitable for probing nanoscopic voids in polymers, molecular solids, soft materials, and bio-media [2–5]. It enables analysis of free volume and its relation to molecular packing, disorder, and composition [3,4].

Despite its long history, interpretation of PALS spectra in organic materials remains challenging. These systems are often disordered, heterogeneous, and built from complex molecular units. Standard models, including the Tao–Eldrup model and its extensions, rely on simplified assumptions such as idealized cavity geometry and uniform electron density, which may not fully represent real organic environments [2–4]. Consequently, extraction of meaningful parameters may be ambiguous, especially for amorphous polymers, composites, molecular solids, and biological tissues [4,5].

This problem is important in view of progress in positronium research and medical imaging. Studies indicate that positronium properties may provide diagnostic information related to molecular structure and tissue environment [5–7]. Understanding positron transport, thermalization, Ps formation, and annihilation in organic matter is therefore needed for fundamental studies and new diagnostic methods.

The main objective of the project is a systematic study of positron and positronium

interactions with organic materials using PALS, with emphasis on the relation between microstructure and positronium formation and decay. The project will combine experimental measurements, data analysis, and modelling to improve interpretation of lifetime spectra in complex organic systems. Selected simple organic molecules may serve as model systems supporting interpretation of results for polymers, molecular solids, soft matter, and bio-organic materials.

Special attention will be paid to disorder, composition, limitations of free-volume models, and methods for extracting reliable physical parameters from lifetime spectra. The molecular-level component may include simplified modelling or comparative analysis based on available tools and literature data. This will help connect molecular properties, such as electron density and chemical composition, with annihilation characteristics in condensed organic systems.

Experimental work will use a fast-fast coincidence ORTEC PALS system with plastic scintillators and PMTs. A key task will be adapting this setup for organic samples and calibrating the modified configuration. Expected outcomes include better understanding of positron and positronium behaviour in organic matter, improved methodology for interpreting PALS spectra, and models relevant to materials science and medical imaging.

### 1.3. Work plan

- (a) Literature review and preparation
- (b) Adaptation and setup calibration
- (c) PALS measurements of selected organic materials
- (d) Analysis and verification of free-volume models
- (e) Molecular-level analysis of simple organic molecules
- (f) Correlation of PALS parameters with material structure
- (g) Interpretation in positronium imaging and medicine
- (h) Dissemination and doctoral thesis preparation

### 1.4. Literature (max. 7 listed as a suggestion for a PhD candidate preliminary study)

- [1] F. Tuomisto, I. Makkonen, *Defect identification in semiconductors with positron annihilation: Experiment and theory*, **Rev. Mod. Phys.** 85, 1583 (2013).
- [2] S. J. Tao, *Positronium Annihilation in Molecular Substances*, **J. Chem. Phys.** 56, 5499–5510 (1972).
- [3] M. Eldrup, D. Lightbody, J. N. Sherwood, *The Temperature Dependence of Positron Lifetimes in Solid Pivalic Acid*, **Chem. Phys.** 63, 51–58 (1981).
- [4] G. Consolati, D. Nichetti, F. Quasso, *Probing the Free Volume in Polymers by Means of Positron Annihilation Lifetime Spectroscopy*, **Polymers** 15, 3128 (2023).
- [5] S. D. Bass, S. Mariazzi, P. Moskal, E. Stępień, *Colloquium: Positronium physics and biomedical applications*, **Rev. Mod. Phys.** 95, 021002 (2023).
- [6] P. Moskal, B. Jasińska, E. Ł. Stępień, S. D. Bass, *Positronium in medicine and biology*, **Nat. Rev. Phys.** 1, 527–529 (2019).
- [7] P. Moskal et al., *Positronium image of the human brain in vivo*, **Sci. Adv.** 10, eadp2840 (2024).

### **1.5. Required initial knowledge and skills of the PhD candidate**

The candidate will develop all necessary knowledge and skills during the project realization.

However, basic knowledge in at least one of the following areas is expected:

- basics in computer programming (preferably Matlab, LabView),
- basic knowledge in electronics, circuits and mechanical design
- basic knowledge in atomic and condensed matter physics

### **1.6. Expected development of the PhD candidate's knowledge and skills**

During the project, the PhD candidate is expected to develop knowledge and practical skills in the following areas:

- positron annihilation spectroscopy and positronium physics,
- principles of matter–antimatter interactions in condensed systems,
- methods for analysing complex experimental data,
- operation, calibration, and optimization of coincidence measurement systems,
- scientific interpretation of microstructural information derived from PALS spectra,
- preparation of scientific publications and presentation of research results.