Summary of Professional Accomplishments
Appendix No. 3
to the application of Dr. Kamil Fedus for conducting the habilitation procedure
in the field of Physical Sciences in the discipline of Physics,
11 May 2017.

1 Name and surname
Kamil Fedus, born 24 January 1983 roku in Kwidzyn (Poland).

2 Scientific degrees:

- 06/2007 **M.Sc.** in Physics: University of Nicolaus Copernicus, Faculty of Physics, Astronomy and Informatics, supervisor - dr Beata Derkowska, title of thesis: *Linear and nonlinear optical properties of Alq$_3$ i DCM.*

- 01/2011 **Ph.D.** in Physics: Universite d'Angers (France), Laboratoire des Photonique d'Angers, supervisor - dr Georges Boudebs, title of thesis: *Development of methods for measuring optical nonlinearities of third order.*

3 Academic positions:

- 02/2011 - 02/2012: postdoctoral fellowship at University of Trento (Italy), Nanoscience Laboratory, investigator in the project *Nonlinear optical properties of strained silicon waveguides.*

- 02/2012 - : adjunct researcher in the Devision of Didactics of Physcis, Institute of Physics, Faculty of Physics, Astronomy and Informatics, University of Nicolaus Copernicus in Toruń (Poland)

4 Awards and scholarships:

- 2014: Senior Advanced Research Award of the Polish-American Fulbright Commission for realization of four months project in laboratory of dr Murtharda Khakoo at California State University Fullerton, USA

- 2013: Scholarship START of the Foundation of Polish Science

- 2013: Scholarship of Polish Minister of Science and Higher Education for outstanding young scientist

5 **Indication of scientific achievement following article 16 par. 2 of act from 14 March 2003 on scientific degrees and scientific title and on degrees and title in arts (Journal of Laws no. 65, pos. 595 with changes):**

A **Title of scientific achievement**
Publication series:

__Study of cross-sections for electron and positron scattering by atoms and molecules in the gas-phase__

B **Author/authors, title, year, publisher**
More detailed contributions are given in separate Appendices, including statements of other co-authors - see Appendix No. 4 and No. 5.

No.	Publication	IF	5-year IF	my contri-bution %
H1	**K. Fedus**, G. Karwasz, Z. Idziaszek, *Analytic approach to modified effective-range theory for electron and positron elastic scattering,* Phys. Rev. A. **88**, 012704 (2013)	2.991	2.598	40%
H2	**K. Fedus** *Electron Scattering from Neon Via Effective Range Theory,* Braz. J. Phys. **44**, 622 (2014)	0.810	0.844	100%
H3	**K. Fedus** *Modified effective range analysis of electron scattering from krypton,* Phys. Scr. **89**, 1 (2014)	1.126	1.086	100%
H4	**K. Fedus**, *Markov Chain Monte Carlo Effective Range Analysis of Low-Energy Electron Elastic Scattering from Xenon,* Braz. J. Phys. **46**, 1 (2016)	1.042	0.844	100%
H5	**K. Fedus**, G. Karwasz, *Ramsauer-Townsend minimum in methane – modified effective range analysis,* Eur. Phys. J. D **68**,93 (2014)	1.228	1.224	70%
H6	**K. Fedus**, G. Karwasz, *Positron Scattering at Thermal Energies,* Acta Phys. Pol. A **125**, 829 (2014)	0.530	0.540	85%
H7	**K. Fedus**, J. Franz, G. Karwasz, *Positron scattering on molecular hydrogen: Analysis of experimental and theoretical uncertainties,* Phys. Rev. A. **91**, 062701 (2015)	2.765	2.598	40%

H8	Jan Franz, **K. Fedus**, G. Karwasz, *Do positrons measure atomic and molecular diameters?*, Eur. Phys. J. D **70**, 155 (2016)	1.208	1.224	40%
H9	**K. Fedus**, *A rigid sphere approach to positron elastic scattering by noble gases, molecular hydrogen, nitrogen and methane*, Eur. Phys. J. D **70**, 261 (2016)	1.208	1.224	100%
H10	**K. Fedus**, C. Navarro, L. R. Hargreaves, M. A. Khakoo, F. M. Silva, M. H. F. Bettega, C. Winstead, V. McKoy, *Low-energy elastic electron scattering from isobutanol and related alkyl amines*, Phys. Rev. A. **90**, 032708 (2014)	2.808	2.598	30%
H11	**K. Fedus**, C. Navarro, L. R. Hargreaves, M. A. Khakoo, A. S. Barbosa, M. H. F. Bettega, *Differential elastic electron scattering by pentane*, Phys. Rev. A. **91**, 042701 (2015)	2.765	2.598	30%
H12	G. Karwasz, **K. Fedus**, *Some Systematics in Electron Scattering Cross Sections*, Fusion Science & Technology **63**, 338 (2013)	0.591	0.680	40%
H13	**K. Fedus**, G. Karwasz, *Electron scattering on molecules: search for semi-empirical indications*, Eur. Phys. J. D, accepted for publication (2017)	1.208	1.224	80%

C **Discussion of scientific goals, results obtained, and their applications:**

5.1   Introduction and motivations

The history of research on the basic physical processes occuring during the collision of electrons with atoms and molecules in the gas phase dates back to the beginning of the 20th century and the famous Ramsauer's experiments [1]. These experiments have shown that, for a certain range of electron kinetic energy, the atoms of heavy noble gases are practically "transparent" to electrons. In other words, the probability of free electron interaction with these atoms is significantly reduced. This phenomenon, known as the Ramsauer- Townsend minimum, has no explanation in classical mechanics and it can be only understood using the theory of matter waves. This result was one of the groundbreaking findings that have established the quantum mechanics as the basic theoretical tool for a description of the microscopic world. Systematic and very extensive studies on the interaction of electrons with atoms and molecules over the past 100 years have contributed to a significant progress in our knowledge about atomic and molecular structures and phenomena occuring on microscopic scale. It is no exaggeration to

say that almost everything we know about the microscopic world is the result of scattering experiments. At the same time, the scientific achievements of this research field are still a source of development of many advanced technologies.

Despite the long history of research on the interaction of electrons with atoms and molecules many issues in this field remain open, especially in the context of the challenges faced by contemporary science and technological projects. These include the development of plasma diagnostic methods in the new generation of fusion reactors [2] and a demand for more precise plasma etching [3] in semiconductor technology. These issues urgently require reliable scattering cross-sections (i.e. probabilities) for direct and resonant partial processes occurring during the interaction of electrons with different atoms and molecules in a very wide electron energy range (from hundredths of eV to several thousand eV). These partial processes include: (i) elastic collisions, (ii) rotational, vibrational and electronic excitations, (iii) ionization and (iv) dissociation phenomena. The precise values of scattering cross-sections for all these processes for a wide range of atoms / molecules are essential as they are used as input parameters for advanced numerical models simulating complicated plasma environment. Two articles [**H12**, **H13**] from the considered publication series were written due to my involvement in the work of the international research group [4] (under the auspices of the International Atomic Energy Agency) aiming to evaluate reference scattering cross sections for molecules that are important in plasma-based technological processes (the official member of this group is Prof. Grzegorz Karwasz, head of my devision). The first article [**H12**] is a review of some semi-empirical dependencies in available cross-sections that may be helpful in constructing reference data. The second article [**H13**] is an attempt to estimate the applicability of the so-called Born approximation for various partial processes: elastic scattering, rotational and vibrational excitations and ionization.

Another important issue that motivates the research on the scattering cross-sections for electron collisions with molecules is related to studies on the physical processes induced in biological matter by ionizing radiation [6]. The understanding of mechanisms repsonsible for a destruction of biological tissues may increase the effectiveness of radiation therapy in the treatment of cancer. The groundbreaking works by L. Sanche and co-workers [5, 6] have shown that the greatest havoc in living cells (including double strand breaks in DNA) does not originate from primary ionisation products - high energy electrons but from secondary products - low-energy particles ($E < 30$ eV). The slow electrons tend to be resonantly attached to the chemical bonds in organic molecules. The resulting negative ions are metastable and their decay is generally accompanied by dissociation of chemical bonds. Research on electron scattering on large organic molecules in the gas phase can provide important information about the position of these resonances and the nature of their formation. In turn, the knowledge of cross sections for all partial processes will allow to create numerical models of electron beam propagation in condensed matter [7]. Electron scattering cross-sections for large molecules are also needed in studies on the hydrocarbon plasmas created during the ignition and combustion of biofuels [8]. I carried out the research on the cross-sections in these contexts in cooperation with Dr. M. Khakoo from California State University Fullerton in USA. The result of this collaboration are four articles from which two of them [**H10**, **H11**] are included in the considered publication series due to my significant contributions. Both works involve the measurements of differential scattering cross-sections in a wide angular (5°-130°) and energy ($1-100$ eV) ranges for polar molecule of isobutanol (C_4H_9OH) [**H10**] and nonpolar molecule of pentane (C_2H_{12}) [**H11**]. In both papers the main objective was to find the presence of resonances in the elastic scattering channel.

One of the most interesting and at the same time the most difficult field to investigate is the low-energy electron scattering, $E < 1$ eV. It is particularly fascinating subject because the de Broglie's wavelength of slow electron can be much larger than the size of studied atoms or

molecules. As a consequence, the main role in collisions is played by the properties of matter waves. So, the scattering of slow ("cold") particles is a very good test for quantum theories. However, the determination of cross sections at low-energies is very difficult, particularly for the *ab initio* theories due to their high sensitivity to the representation of short-range (multi-body in nature) correlation effects between the incoming particle and the electron cloud of the target. On the other hand, the measurements of cross-sections in low-energy are relatively scarce due to the technical difficulties related to the formation of stable monoenergetic electron beam characterized by high resolution. So far, the best available experiment comes down with energy to 10 meV [9, 10]. As a result of these problems, there are many discrepancies between theoretical and experimental scattering cross-sections, especially for polar molecules (e.g. for H_2O the discrepancies between the various data are even over 100%). An alternative approach to the problem of low-energy scattering is the determination of cross-sections using the "extrapolation" to zero energy of reliable experimental data measured at high energies. This approach is based on the Modified Effective Range Theory (MERT), which was proposed in the 1960s [12]. However the applicability of this method in its original form was strongly limited to very low energies $E << 1$ eV [13]. At low energy regime there are virtually no available experimental data to be extrapolated. In 2006, Idziaszek and Karwasz [14] proposed an alternative version of this method allowing for an extension of its applicability to much higher energies, where much more experimental datastes are available. In the considered publication series, in works [**H1, H2, H3, H4, H5**], the applicability of new MERT has been deeply verified and used to determine cross-sections for low-energy electron scattering by all noble gases and several simple molecules.

The study on positron (anti-electron) scattering cross-sections is the concurrent (to electron collisions) subject included in the considered publication series. The experimental research on positrons collisions with atoms and molecules was already undertaken in the 1970's [16], but only recently the new positron sources and moderators [17, 18, 19] have expanded the scope of studies for new molecules and much wider energy ranges. Positrons are an alternative probe to electons of the microscopic world properties. Among the most fundamental uses of positrons are the formation of the anti-hydrogen [20], the possibility of producing Bose-Einstein condensate on the positronium molecule [21] and the possibility of generating positron plasma [22]. In astrophysics the positron annihilation signal is a very important diagnostic tool to study phenomena occurring in the interstellar matter [23]. In particular cross-sections for many atoms and molecules may help explain the sources of the strong annihilation signal recorded from the center of the galaxy [24]. Positron annihilation is also used to study defects and structural changes in condensed matter [25] (including the positron lifetime spectroscopy, which I am also using in my scientific work [**P5, P6, P7**], see the section *Other scientific activities*). Positrons also have a number of technological applications including the most well known one - the Positron Emission Tomography [26]. Accurate understanding of positron interaction with matter requires precise knowledge of scattering cross-sections for the most fundamental partial processes occurring during collisions of positrons with atoms and molecules.

One of the most fundamental problems undertaken in this series of publications is the study of differences observed in electron and positron cross-sections. For very high impact energies ($E >> 100$ eV), the total cross-sections for both particles converge [27] since the fast particles cause little deformation of the electronic cloud in target (the latter can not keep up with the changes of particle position). This weak interaction can be described in the Born approximation according to which the cross-sections are independent of the charge sign. On the contrary a significant differences appear in lower energies ($E << 100$ eV) where polrization forces play a dominant role. First of all, for positrons there is a new scattering channel associated with the positronium formation, i.e., the bound state of $e^+ - e^-$ (hydrogen-like atom), which ultimately decays in the annihilation process. The positronium formation is the lowest inelastic process

in the energy scale for many light atoms. Another difference between electrons and positrons are completely different energy dependencies of scattering cross-sections for energies below the positronium formation threshold. This is due to two reasons: (i) the difference in the nature of static interactions: attractive for electrons and repulsive for positrons and (ii) the lack of exchange interaction for positrons. Consequently, the short-range correlation effects in positron - target collisions play a much more important role than for electrons. These phenomena are so strong that they can lead to the formation of virtual positronium [28, 29] - a very strongly correlated pair e^+e^- moving temporary in the field of positive ion. Formation of a virtual positronium in the elastic scattering channel is still only a theoretical hypothesis that has no direct confirmation in the experiment. Nevertheless the inclusion of this effect in theoretical calculations has greatly improved the agreement of the theories with avaiable experimental results for noble gases [28, 29]. In the work of [**H7**] the problem of presence of a virtual positronium in positron - molecular hydrogen (H_2) collision is discussed through the comparative study of experimental data, DFT calculations (not taking into account this effect) and MERT analysis (formulated for the first time within the frame of Bayesian statistics). The MERT analysis has been also applied for positron cross-sections in [**H1**] in order to check the aplicability of this model for positron scattering. In addition, in [**H6**] it has been shown that MERT may be useful for a description (parameterization) of scattering sections for annihilation of positrons at thermal energies (when probability of annihilation is very high). In the same paper it has been also shown that MERT allows for a construction of a "bridge" between two qualitatively different experiments: attenuation methods determining elastic scattering cross-sections and annihilating experiments determining positron binding energies to large organic molecules [30].

The inclusion of virtual positronium in theoretical calculations allows to reproduce a flat part of total scattering cross-sections appearing just below the real positronium threshold for many atoms and molecules (eg, Ar, Kr, H_2, N_2, CH_4). Karwasz [31] noticed that the constant value of cross-sections in this "flat" part scales in the same way as the "dimensions" of atoms and molecules. In other words, the virtual independence on collision energy suggests that positrons behave as they would be scattered by a rigid sphere. However, the quantum model of a rigid sphere does not reproduce the values of measured cross-sections [32]. In paper [**H8**] this hypothesis was verified in more quantitative way by comparing experimental cross sections with theoretical "radii" of atoms and molecules (van der Waals and covalent radii). In addition a similar scaling was studied in paper [**H9**] using a simple potential model of infinitive barrier (i.e. the rigid sphere) combined with long-range polarization potential ($\sim r^{-4}$).

To summarize, a significant increase of computing power over the past decade allows for a progress in numerical implementation of various theoretical models describing complicated multi-body effects in electron and positron collisions with atoms and molecules. Unfortunately, these advances are not accompanied by the convergence of cross-section results obtained by various methods. Consequently, the problem for an estimation of uncertainties in theoretical calculations of atomic and molecular data becomes an important issue since the computed results are frequently used as the primary source of data for input into modeling codes [33, 34]. In addition, the most advanced contemporary theories involve such large basis sets and complicated equations that they are not easily applied to each specific molecule for which data are urgently needed. Hence, in addition to experimental measurements, the semi-empirical analysis of angular and energy dependencies of scattering cross-section becomes important. The main goal of the present publication series was to study the scattering cross sections for different partial processes occurring in the collisions of electrons and positrons on atoms and molecules in the gas phase using semi-empirical methods and experiment. These studies, in addition to proposing reliable cross-section datasets, also aimed at deepening the understanding of the nature of the most fundamental processes occurring during the scattering - particularly in the low energy regime.

5.2 Determinations of scattering cross-sections at low energies using the modified effective range theory

Modified Effective Range Theory (MERT) was proposed by O'Malley et al. [12] to describe elastic scattering of light charged particles (electron, positron) by nonpolar atoms and molecules as an extension of the Efective Range Theory (ERT). The latter is commonly used to interpret scattering results in low-energy nucleon collisions: neutron-proton or neutron-neutron. ERT describes the problem of scattering in the language of partial waves, i.e. the eigenfunctions of angular momentum operator, which decomposes the total wave function of the colliding system of particles. The method allows to express the phase shifts of partial waves induced by collisions as a function of kinetic energy of particles and some empirical parameters (known as the effective range parameters). ERT is based on the premise that interaction between particles is short-range in nature, in other words colliding particles "feel each other" only at short distances. This assumption can not be applied to the electron (or positron) scattering on atoms because of the presence of long-range (theoretically extending to infinity) polarization potential ($\sim r^{-4}$). O'Malley et al. [12] showed that in the presence of this potential, partial wave phase shifts could be also expressed as a function of energy using similar expressions as in the ERT approach for nucleons. In the proposed model, the interaction potential between the incident particle and the non-polar atom is divided into a long-range part ($\sim r^{-4}$) and a short-range part. The final relations are obtained by solving analytically radial Schrödinger equation with pure polarization potential. Short-range effects are taken into account by imposing appropriate boundary conditions for analytical solutions (so called Mathieu functions). The MERT theory has gained great popularity as a basic tool for an analysis of low-energy experimental data and it has been frequently used to extrapolte experimental results to the zero energy and near zero scattering angles, i.e. the regions hardly accessible experimentally. Moreover it has been frequently used to estimatie the scattering length (A) - one of the most important physical quantities in the quantum scattering theory. The scattering length is directly related to the elastic scattering cross-section at the zero energy: $\sigma(0) = 4\pi A^2$. This quantity informs not only about the "strength" of the interaction but also about its nature. Positive A indicates the possibility of a bound state (particle - atom) in very low energy regime. On the other hand, large negative A indicates the possibility of a "virtual" state formation [35] .

Unfortunately, the applicability of the original version of MERT is limited to very low energies - Buckman and Mitroy [13] proved that MERT is valid for $E << 1$ eV in the case of noble gases. There are few experimental data in low energy regime and those available are generally characterized by large errors. This strongly limits the reliability of the MERT extrapolation and obtained scattering parameters. In 2006 Idziaszek and Karwasz [14] proposed an alternative approach to the model which extends the applicability of MERT to higher energies. Unlike the original version of the theory, the new approach uses the full analytical form of the solutions of the Schrödinger equation with the potential r^{-4} while the effective range approximation is exclusively applied to the short-range part of the interaction potential. Idziaszek and Karwasz used the new MERT approach to briefly analyze scattering cross-sections for positron - argon [14] and electron-nitrogen collisions [15] by comparing the model with subjectively selected experimental data. However the applicability of new MERT approach has not been verified in more systematic and extensive way.

In [**H1**] I verified the applicability of the new approach to the modified effective range theory (MERT) proposed by Idziaszek and Karwasz [14]. For this purpose, I applied the model to several alternative experimental total cross sections (TCS) describing electron and positron scattering on helium (He), argon (Ar), molecular hydrogen (H_2) and methane (CH_4). TCSs provide a good basis for analysis since they are measured in absolute and very precise way in the beam

attenuation experiments. For electrons, I have chosen two validation criteria for estimating the correctness of derived effective range parameters: (i) the continuity of partial wave phase shifts as a function of energy and (ii) the agreement between the model and experimental differential cross-sections (DCS) measured in cross-beam exeriments and momentum transfer cross-sections (MTCS) derived from swarm experiments. As a result of this extensive comparative study, I have shown that the new approach to MERT has the potential to describe elastic scattering cross-sections for e^-+ He, e^-+ Ar and e^-+H$_2$ in very wide energy ranges: from the zero-energy up to the ioniztion thresholds. For example, in the case of helium, the range of applicability of the model was estimated to be 0 - 20eV!.

In addition, in article [**H1**] I have shown that MERT can be used as a diagnostic tool for the analysis of the reliability of the measured cross-sections. This analysis consists in checking the compatibility (in the terms of scattering phase shifts) of elastic cross-sections measured by beam attenuation methods, differential cross-sections measured by cross-beam techniques and momentum transfer cross-sctions determined from swarm experiments. In particular I have shown that the latest measurements of elastic cross sections for Ar carried out for the first time in the ultra-low energies (down to 10 meV) [9] are likely to be underestimated as they do not agree with all other types of available cross-sections.

In the articles [**H2,H3,H4**] I continued the MERT analysis from [**H1**] for noble gas atoms by studying electron collisions with neon [**H2**], krypton [**H3** and xenon [**H4**]. The goal of these analyses was to propose coherent and compatible sets of elastic, differential and momentum transfer cross-sections ranging from the zero energy up to the ionisation thresholds. In addition to the recommended cross-sections, the most important results of these three papers are the most probable values for electron scattering lengths (A). The latter quantities were determined using for the first time an innovating MERT fits that take into account most of the available experimental datasets. To achieve this goal an algorithm for simultaneous MERT fits to the series of different experimental datasets was developed. As a result I have shown that for neon the value of $A = 0.227a_0$ (Bohr units) is consistent with recent calculations by Cheng et al.[36], for krypton $A = -3.486a_0$ confirms the results of the old MERT analysis done by Weyhreter et al. [37], while for xenon the most likely value is $A = -6.51a_0$. It should be noted that for the last atom there exists in the literature a very large discrepancy between the scattering lengths determined by different methods. This refletcs a high sensitivity of scattering calculations in the low-energy region for xenon to the representation of the short-range correlation potential. Summury of MERT analisys for all noble gases [**H1,H2,H3,H4**] is the linear relationship between the scattering length (A) and the static polarizability of atoms (α): $A \approx -0.29\alpha + 1.4$ [**H4**]. Such dependency was studied in details in [38, 39] without achieving the final conclusions about the close form relation between A and α.

In the work [**H1**] I estimated the MERT applicability for a description of e^-+CH$_4$ collisions to the energy range 0 - 2 eV (where Ramsauer-Townsend minimum is present). The limitation of the model's applicability to such low energy is most likely due to the presence of resonant vibrational excitation in the range of $E > 2$ eV [40] (there is still no sufficient experimental proves for theoretical predictions). The presence of strong resonance effects in the vibrational channel can significantly affect elastic scattering as a result of a channel coupling - an effect that is not included in the MERT. In [**H1**] two available experimental sets of total scattering cross sections (TCS) [41, 42] were considered as the basis for the analysis. Since the contribution of the vibration excitation to TCS is significant in the region of Ramsauer-Townsend minimum of CH$_4$, to analyze elastic data the vibrational cross sections (VCS) must be subtracted from TCS. We arbitrarily choose the VCS by Schmidt [43]. However it must be emphasized that there is no consensus in the literature on VCS in the considered energy range, see [43, 44, 45, 46, 47]. In addition you can find different VCSs proposed by the same authors in different papers [44, 45, 47].

The difficulty in estimating VCS is due to the threshold nature of vibrational excitation in the region of Ramsauer-Townsend minimum. This results in high sensitivity of calculations to the choice of numerical models. In work [**H5**] I carried out a more detailed analysis of the elastic and vibrational cross-sections for methane. Unlike [**H1**] as a basis for analysis I used the latest elastic differential cross-section (DCS) measured with extremely high energy resolution over wide angular range at 45°, 90°, 135° and 180° [48] (results were obtained using the innovative magnetic angle changer technique used in the cross-beam scattering experiment). In order to optimize the analysis, a procedure for the simultaneous fit of the model to all four considered data sets was developed. The derived scatering phase shifts allow to propose a set of recommended cross-sections for elastic scattering in the considered energy range. Comparison of elastic cross sections with experimental TCS allowed to estimate VCS. The latter was found to be in great agreement with the theoretical results published by Altorpe et al.[44]. For verifying the correctness of recommended elastic and vibrational cross sections, both datasets were used to calculate the swarm transport parameters (drift velocity and transverse diffusion coefficient) from the Boltzmann transport equation. The derived parameters were found to be in great agreement with the results of swarm experiments. To summarize, the main achievement of work [**H5**] is the proposition of recommended elastic and vibrational cross-sections for electron scattering from methane in the region of Ramsauer-Townsend minimum.

In the case of positrons, determining the correctness of the effective range parameters is much more difficult than for electrons. First of all, the divergences between available (and much less numerous) experimental total cross-sections (TCS) are much higher. Moreover the measurements of differential cross-sections (DCS) are still very scarce and swarm experiments have not been realized yet (despite intensive theoretical works in this direction [49]). Nevertheless, the MERT analysis carried out in [**H1**] showed that the fit of the model to most available experimental data (for He, Ar, H_2 and CH_4) allows to obtain the continuous phase shifts of partial waves as a function of energy that are in good aggrement with some theoretical results. The exception are TCS by Zecca et al. [50] for H_2 for which no satisfactory fit was achieved. A similar result was given by MERT's predictive analysis within the frame of Bayesian statistics in [**H7**] where the traditional fitting method was replaced by the Monte Carlo numerical technique. Indeed, in the latest paper of these authors [51] their experimental data for H_2 were corrected due to the angular resolution error. In this way the correctness of the analyzes carried out in [**H1**, **H7**] was confirmed. Knowledge of reliable cross-sections for molecular hydrogen is particularly important since as the simplest molecular object it can be a benchmark for quantum theories. Moreover the positron cross-sections for H_2 are important for modeling the propagation of positrons in interstellar matter [24]. Unfortunately, there is a large discrepancy between the three latest experimental datasets on TCS: Karwasz et al.[53], Zecca et al.[50] and Machacek et al.[54] in the energy range below the positronium formation threshold ($E < 10$ eV). On the other hand, the theoretical work by Mitroy and co-workers [55] allowed to derive a very reliable average value of the scattering length $A \approx -2.63a_0$ (in Bohr units) for this molecule. This result should be regarded as trustworthy since the theoretical method used for its determination has solved the long-standing discrepancy between experimental and theoretical cross-sections for positron annihilation on the H_2 molecule in the thermal energy range. In the work [**H7**] I showed that except for data by Zecca et al. [50], the other two experimental results [53, 54] are compatible with Mitroy's scattering length. The latest theoretical results [51] seem to be in better agreement with TCS by Karwasza et al. [53] [**H7**].

One of the most fundamental issues discussed in research on the positron scattering from atoms and molecules in the gas phase is the existence of Ramsauer-Townsend minimum (in the language of partial waves this corresponds to the sign change of s-wave phase shift) [52]. The MERT analysis in work [**H1**] has undoubtedly confirmed the presence of this effect despite

the fact that this minimum is not visible in TCS for Ar, H_2 and CH_4. This unusual situation when compared to electrons is due to the different nature of positron - atom interaction - the repulsive nature of static interaction, the absence of exchange forces and the presence of very strong correlation effects (virtual positronium). As a consequence the s-wave phase shift reaches zero for relatively high energies ($E > 1$ eV) where the contributions of higher partial waves (p and d) to TCS are significant (smoothing the elastic cross sections).

The ultimate fate of every positron is an annihilation with the electron, that is, the destruction of both particles and the conversion of their energies to gamma rays. Experimental results and theoretical calculations show a close relationship between scattering cross sections for elastic collisions and direct annihilation. Namely, the increase of elastic cross sections with decreasing energy is accompanied by a significant increase in the probability of annihilation. This close relation is observed for noble gases and small non-polar molecules (e.g. N_2, H_2, C_2H_4) [56]. For both processes, the increase of cross-sections in the low energy regime is a consequence of the increasing role of the long-range polarization potential ($\sim r^{-4}$) and the strong nature of the short-range correlation effects. The strong polarization forces are responsible for an increase of the electron density near the positron position resulting in larger chance for elastic scattering or annihilation. Gribakin [56] proposed a simple relation (with empirical parameters) which allows an estimation of annihilation cross sections using the partial wave phase shifts induced by elastic collisions. In paper [**H6**] I showed for Ar and N_2 the combination of MERT with the model proposed by Gribakin [56] allows to describe cross sections for elastic collisions and annihilation in the thermal energy range using several parameters.

Paper [**H6**] deals also with the problem of compatibility between the positron binding energies to large organic molecules (C_6H_6 and C_6H_{12}) measured in annihilation experiments [30] with the experimental results of elastic cross-sections measured with the attenuation technique [57]. Annihilation experiments carried out by C. Surko and co-workers [30] with elaborated positron trap method revealed the resonance enhancements of the annihilation process for large organic molecules in low energy regime. Since the resonant energies are closely correlated with the vibrational excitation energies the mechanism of Vibrational Feshbach Resonances (VFR) has been proposed to explain the experimental findings [30]. According to this model when the positron has just the right energy, it can excite a vibrational quantum in a molecule and drop into a bound state. Once in the bound state, the resulting increase in the overlap of the positron wave function with those of the molecular electrons results in a greatly enhanced annihilation rate. The experimentally observable shifts of the anihilation resonance peaks with respect to the position of vibrational excitations (determined from the infrared absorption spectra) correspond, in accordance with the model, to the positron binding energies. The binding energy is directly related to the scattering length (i.e. to the elastic cross-section for the zero energy): $E_b \approx 1/(2A^2)$ [30]. The MERT analysis published in [**H6**] shows that it is possible to achieve a good fit of the model to the elastic cross sections of Ref. [57], which is compatible with the scattering length determined from the annihilation experiments [30]. In this way, the scattering cross-sections for benzene and cyclohexane have been proposed in low energy range that are consistent with two qualitatively different experiments. It should be added that all the theoretical calculations of the elastic cross-sections for C_6H_6 [58, 59] are significantly lower than available experimental data.

In paper [**H6**] only a positive scattering length (A) was assumed in the MERT analysis since $A > 0$ indicates the existence of the bound state (following the picture of Vibrational Feshbach Resonances). However the positron binding energy depends on the square A, so the scattering length can be also negative - indicating the presence of a virtual state that may also lead to the enhancement of annihilation (then the mechanism responsible for resonant anihilation would be different from Feshbach's resonances). In article [**P7**] this possibility is also taken into account

and an alternative set of cross-sections for both molecules are derived. Verification which of the datasets (with positive or negative A) are closer to the truth belongs to the experiment and more advanced calculations. The work [**P7**] is not included in the considered publication series because it is published in a journal that does not have an impact factor.

5.3 Cross-sections for scattering of low-energy positrons: mechanisms of scattering, virtual positronium, interaction potentials

For H_2 between $3 - 10$ eV the energy dependence of total cross-sections for positron is almost "flat" (virtually independent of energy). In this range almost all available theories predict lower cross-sections than available experimental data. These discrepancies could be explained by the lack of virtual positronium formation [28] in all theoretical approaches. The latter effect is a manifestation of a very strong correlation between positron and electrons of the target. The latest CCC (Convergent Close Coupling) calculations [51] require the use of as many as 1013 pseudo-states of hydrogen molecule to reproduce some experimental cross sections. Such powerful calculations are also needed to reproduce the Mitroy's scattering length [55] which should be treated as a reference point in the analysis of the scattering cross-sections for H_2. The use of lower number of states in the same CCC method [60] underestimates the scattering length and cross-sections in the "flat" part. An additional confirmation of the presence of very strong correlations in $e^+ + H_2$ collisions between $3 - 10$ eV is provided by DFT calculations published in [**H7**]. These calculations do not take into account the virtual positronium phenomenon and consequently they are much lower than experimental data. Interestingly, in the same work I showed using MERT that the total and differential cross sections published in Ref.[54] are compatible with each other in the range of $3 - 10$ eV. This result suggests that MERT is able to take into account the contribution of the virtual position to the scattering cross-sections within the frame of used parameterization of short-range effects.

A similar effect of "flattening" of the total scattering cross-sections just below the threshold for the real positronium formation is observed for many other atoms and molecules (e.g. Ar, Kr, N_2, CH_4). Karwasz [31] noticed that the constant value in the "flat" part scales in a similar way as the "geometric" dimensions of atoms. In other words the scattering cross-sections behave in the same way as if the positrons were scattered by a rigid sphere. However the quantum model of rigid sphere is not able to reproduce the measured values of cross-sections [32] because it does not take into account the strong polarization effects leading to the formation of a virtual positronium. The decisive role of these effects is shown by the DFT calculations published in [**H8**] - using a similar approach as in [**H7**]. However, unlike for H_2 this time DFT was able to reproduce "flat" parts of cross-section energy dependencies for all studied targets (i.e. Ar, Kr, N_2, CH_4). It was achieved by including higher order terms ($\sim r^{-4}, \sim r^{-6}, \sim r^{-7}, \sim r^{-8}$) in the multipole expansion of long-range polarization potential. Inclusion of these additional term allows to compensate the lack of virtual positronium in short-range interactions - the neglection of these terms leads to underestimation of the cross-sections with respect to the experiment (as for H_2). On the basis of these results and conclusions, the picture of rigid-sphere like scattering from Ref. [32] was redefined in [**H8**] to the picture of "sticky ball" scattering as the positron "stick" to the atom in the process of virtual positronium formation . Due to the presence of a strong repulsive static interaction, the positron does not penetrate deeply into the atomic structure and it interacts effectively only with the valence electrons. This type of interaction resembles qualitatively a covalent bonding. In [**H8**] it was shown that the values of the total scattering cross-sections (σ) in the "flat" part of energy dependencies for Ar and Kr are compatible with the covalent radii (r_c) of these atoms estimated from crystallographic data when using a simple relation: $\sigma = \pi r_c^2$. This result confirms the correctness of the proposed picture

of a "sticky ball" to explain the presence of a "flat" part in cross-section energy dependence. An additional argument confirming the postulated scattering mechanism is the observation that the matching points between the long-range potential and the short-range correlation potential in DFT calculations [**H8**] correlate with van der Waals radii of atoms (estimated at X-ray diffraction). The van der Waals radius corresponds to the dimension of the spherical space occupied by the atom, which is inaccessible to other atoms. In other words, it corresponds to the largest distance from the atomic nucleus on which the atom can still be treated as a single object (without internal structure). From the point of view of the incident positron, the van der Waals radius should correspond to the shortest distance of the positron from the nucleus, where the long-range polarization potential is still dominant over the short-range effects.

For decreasing positron energy, farther away from the threshold for real positronium formation, scattering cross-sections are not constant any more since their values are rapidly growing. This can be explained by the fact that as the energy is lower the long-range polarization potential becomes more important and the scattering occurs at larger positron-atom distances. Consequently, the contribution of (short-range in nature) virtual positronium becomes less significant. Nevertheless, this contribution is not negligible as evidenced by the scattering lengths for positrons which absolute values are much higher than those for electrons.

In the paper [**H9**] I attempted to explain the energy dependencies of total cross-sections (for noble gases and H_2, N_2, CH_4) in the range from the zero energy up to the thresholds for the real positronium formation using a simple potential model of rigid sphere (infinite potential barrier) combined with the long-range dipole polarization potential ($\sim r^{-4}$). The infinite potential barrier approximates the repulsive static interaction while the potential r^{-4} is supposed to approximate the attractive correlation and polarization effects. The proposed numerical model is based on the Mathieu functions - the analytical solutions of the radial equations Schrödinger equation with the potential r^{-4}. There is only one parameter in the model, the radius of rigid sphere, that has to be determined empirically.

Such a simple potential model does not capture the full behavior of the positron - atom interaction, but it was found to reproduce quite well the scattering cross-sections as a function of positron energy. First of all, the model confirmed that the "flat" part of the cross-section scales with the dimensions of atoms - in this case with the radius of rigid sphere. Furthermore, it was found that rigid sphere radii are compatible with the positions of principal maxima in the radial distribution of outermost atomic orbitals. Moreover the model reproduces scattering cross-sections for targets characterized by moderate dipole polarizabilities (Ar, Kr, H_2, N_2) in good agreement with experiments for impact energies covering almost entire range from the positronium formation threshold down to the zero energy!

The analysis of the model's applicability has led to some other interesting conclusions. Reproduction of experimental results requires very deep polarization potential, more than tens of eV below zero (e.g. -49eV for Ar). On the other hand more realistic potentials [**H8**], [61] obtained with more advanced models for short-range effects, are characterized by a minimum of a few eV below zero. In other words, a very strong potential r^{-4} is needed in order to compensate the absence of short-range positive correlation effects (including virtual positronium) when the static repulsion is modeled by an infinite potential barrier. This result also indicates that it is possible to construct any semiempirical model for positron-atom elastic collisions as long as the long-range polarization potential is included. The most interesting result, which requires separate research, is that a small change in rigid sphere size allows to reproduce the various theoretical results available in the literature. Saying it differently, the shift in the position of infinite barrier gives exactly the same effect as using completely different representations for short-range interactions.

5.4 Cross-sections for scattering of low-energy electrons by large organic molecules - experimental measurements

The problem of low-energy electron scattering from large organic molecules has been undertaken by me in colaboration with Dr. M. Khakoo from California State University in Fullerton (USA) and the results of this cooperation are described in papers [**H10**, **H11**, **P9**, **P10**]. A four-months mid-term stay financed by the Fulbright Commission allowed me to carry out experimental studies of differential elastic cross sections for selected organic molecules in a wide angular $(5^o - 130^o)$ and energy $(1 - 100$ eV$)$ ranges. The experiments were performed using an electron energy loss spectrometer combined with the relative flow technique [62]. In all four papers [**H10**, **H11**, **P9**, **P10**] experimental results were supported by theoretical calculations using Schwinger multichannel method (SMC) [63]. The SMC method is a modification of Julian Schwinger's variational method [64] for multi-particle systems.

Paper [**H10**] reports a detailed characterization of the differential scattering cross sections (DCS) for the polar molecule of *iso*-butanol (C_4H_9OH) in the full available angular and energy ranges. Moreover the results for its isomer *n*-butanol are also reported in the region of shape resonance in the elastic scattering channel (about 10 eV). The main motivation for this experimental study were SMC calculations [65] carried out for both isomers which revealed different partial wave contributions to the shape resonance. For *n*-butanol, which is a linear molecule, DCS are characterized by a minimum at the scattering angle $\theta = 90^o$ in the resonance region suggesting the dominant contribution of f-wave. On the other hand, for *izo*-butanol, which is a branched molecule, the calculations give a maximum of DCS at $\theta = 90^o$ suggesting a dominant contribution of d-wave. These theoretical results follow the trend observed for many other molecules: the f-pattern for the straight-chain molecules [66, 67, 68, 69, 71] and the d-wave pattern for branched systems [68, 70]. Despite an obvious relationship with the geometry of the molecule, the exact reason of the observed differences is not clear. One hypothesis says that the scattering pattern may be determined by the local symmetry of C–C antibonding orbitals that temporarily trap the projectile to form shape resonances; however, it remains unclear why the C–C antibonding orbitals are more important than the C–H orbitals in determining the scattering pattern [65]. Certainly, the functional groups attached to the main hydrocarbon backbone does not affect the shape resonance, as shown by the calculations for *izo*-butylamine (C_4H_9 NH_2) [**H10**] (in other words, the dipole moment of molecule does not play a role in this effect). A second possibility is that the primary determinant of d versus f-wave scattering is simply the spatial extent of the molecule. Branched systems are more compact than their corresponding straight-chain isomers, making it more difficult, at a given energy, for f waves to penetrate the angular momentum barrier and reach the region of the molecular potential.

Paper [**H10**] reports for the first time the experimental observation of maxima and minima in DCS at $\theta = 90^o$ in the shape resonance region for two isomers. In this way the theoretical predictions were finally confirmed. Previous experimental studies [69, 70] did not reveal these differences due to too low counting statistics. Generally, the maxima at $\theta = 90^o$ for branched molecules are relatively small and very large statistics is needed in order to detect them experimentally. In addition, the measured [**H10**] maxima are lower than the theoretical predictions due to the finite energy resolution of the experimental system.

Paper [**H10**] reports also integral elastic and momentum transfer cross-sections estimated from experimental DCS. To the best of my knowledge these are the first experimental results of the elastic scattering cross sections obtained experimentally for the *izo*-butanol molecule. Comparison of the SMC theory with the experiment shows that medium and large angle scattering is dominated by short-range effects, but the most effective scattering occurs at very low angles (nearly 0°) due to the dominating influence of the long-range dipole potential ($\sim r^{-2}$). For

low energies and small angles, measured DCS are well described by formula derived within the Borna approximation. The problem of the applicability of this approximation is discussed in detail in the work [**H13**] included in the considered publication series.

Paper [**H11**] describes the characterization of DCS for nonpolar n-pentane (C_5H_{12}). Similar to other molecules characterized by linear geometry, the minimum of DCS was observed at $\theta = 90^o$ in the shape resonance region. This is the further confirmation of the trend described in paper [**H10**] - the dominant f-wave pattern for the straight-chain molecules. To the best of our knowledge, measurements from [**H11**] reports for the first time DCS for C_5H_{12}. Despite this work there are also experimental measurements of the total cross sections (TCS) reported by Kimura et al. [72] and momentum transfer cross-sections (MTCS) derived from the analysis of swarm experiments [73].

Few interesting conclusions can be drawn from the comparision of DCS for C_5H_{12} with the available results for shorter molecules from the same alkane family C_nH_{2n+2}: methane, ethane, propane and butane. It appears that in the energy range of $3-100$ eV DCS for all these molecules are characterized by the same angular dependencies. In addition, there is a systematic increase in values of DCS with the length of the alkane chain. Such observations suggest that the electron interacts effectively only with the segment of alkane chain containing two or three carbon atoms. The longer chain only increases the number of scattering centers raising the average value of cross-sections.

All molecules from family C_nH_{2n+2} are characterized by a decrease of TCS starting from the resonance maximum at about 10 eV down to the energies of the order of tens meV, where the SMC theory and analysis of swarm experiments [73] suggest the presence of Ramsauer-Townsend minimum. In the case of C_5H_{12} the results of experiment from [**H11**] shows an existance of additional broad peak in TCS (with a maximum at about 0.4 eV), which is not observed for shorter molecules. The presence of this maximum suggests the existence of a short-lived resonance not predicted by SMC theory. Moreover the TCS measurements in [72] also do not reveal the presence of this effect. The confirmation of this resonance requires further independent experimental and theoretical checks.

5.5   In the search of systematics in scattering cross-sections

Two papers [**H12**, **H13**] from the considered publication series are the results of my involvment in the work of the international research group [4] aiming to establish internationally agreed reference cross-sections for plasma modeling. Both papers have a review nature and concern on the search for systematic dependencies in cross sections that may be useful in constructing reference data using divergent results. Both articles have been prepared for the plasma science community, whose main research activities are related rather with the use of ready-made data than with the cross-section determination.

Paper [**H12**] discusses analogs in total and partial cross-sections for different direct and resonant processes: elastic scattering, rotational excitation, vibration excitation, electron excitation, electron attachement and dissociation processes. This work highlights the most important similarities and trends observed in cross-sections for different molecules depending on dipole moment, polarizability and chemical composition. In addition, a semi-empirical method is proposed for the determination of partial cross sections. This method is based on the estimation of the relative contribution of every single channel to TCS. The applicability of this method in the region of shape resonance for three molecules with the same number of valence electrons: N_2O, CO_2 and OCS is discussed in order to evaluate the contribution of electron attachement. In general, the work [**H12**] indicates the most important points that has to be considered in the critical construction of the reference data.

Paper [**H13**] analyzes the applicability of the Born approximation [35] to the description of scattering cross sections for different partial processes that may occur during electron collisions with polar molecules. The Born approximation assumes that the total wave function of the electron-molecule system is weakly perturbed by the scattering process, in other words, there is a negligable difference between the incident and scattered wavefunctions. Such an assumption is valid only for a weak scattering, which generally occurs during high-energy collisions when the molecule is unable to keep up with changes in the position of the fast particle. Therefore the Born approximation is mainly applied for high-energy channels such as electron excitations and ionizations [74]. The Born approximation is also applicable for threshold regions of rotational and vibrational excitations [75] and low-angle and low-energy elastic scattering on polar molecules when the interaction is governed by long-range forces. Generally it is expected that the Born approximation describes well differential cross-sections (DCS) for all mentioned processes in near zero scattering angle ($\theta \approx 0^o$). However the applicability of this approximation to the integral cross-sections (DCS integrated over entire angular range $0 - 180^o$) is not well studied. Paper [**H13**] is an attempt to assess the suitability of this approximation using the latest experimental data.

The comparison of the Born-formula for elastic DCS with the latest measurements for some polar molecules [76, 77] [**H10**, **P9**] shows a very good agreement between theory and experiments in a very wide angular and energy ranges. For example, for H_2O and energies $E < 4$ eV the Born model agrees with experimental DCS in the angular range $0-130^o$ [76]! The measurements show that as the electron energy increases, the applicability of the Born-formula is getting confined to narrower angular range near the zero angle.

In [**H13**] I also showed that the Born approximation can be used to describe the low-energy ($E < 1$ eV) momentum transfer cross-sections (MTCS) derived from the analysis of swarm experimental data. I noticed however that this conclusion is valid when we take into account MTCS containing the contribution of both elastic and rotational scattering. On the other hand when one separate both channels, the pure elastic MTCS is no longer described by the Born-formula if the rotational excitations are important.

Direct measurements of scattering cross-sections for rotational excitations of polar molecules are very scarce due to technical difficulties associated with the experiment. The excitation energies associated to rotational levels are so low and the angular distribution of scattered electrons is so peaked in the forward direction that experiments do not have enough energy and angular resolution to distinguish elastic and rotational processes. As a consequence, experimental errors are large. However, in [**H13**] it was showed that the avaiable experimental DCS for HCl [78, 79] remain in very good agreement with the Born-formula in very wide angular ranges for low energies ($E < 5eV$).

The situation looks very similar for the vibrational excitations. For a long time there was not enough experimental data to verify the Born's approximation applicability. It was only recently that first direct measurements of integral cross-sections were performed on the asymmetric stretching mode of CF_4 molecule [80]. The results were found to be in very good agreement with the Born-formula. This optically active mode is characterized by very effective charge-transfer between C and F atoms. This results in very strong change of the dipole moment during oscillations. Consequently, there is a very strong long-range dipole coupling between vibrational mode and the incoming electron. This in turn makes the electron scattering effective at large distances (the scattering is weak). It is confirmed by the measurements of DCS for the considered CF_4 mode showing a rapid increase of cross-sections at low scattering angles [81]. On the other hand the short-range effects that are not described by the Born-approximation may significantly affect electron interaction with molecules characterized by much lower transition dipole moments. This is the case for the strongest optical modes of water molecules, as shown in [**H13**].

Paper [**H13**] deals also with the problem of the applicability of the Binary-Encounter-Bethe (BEB) model [82] for a description of partial cross-sections characterizing the production of specific ions in dissociative ionization. BEB is a parameter-free model formulated within the Born approximation, which proved to be very effective in describing total cross sections (a sum of all partial CS) for the ionization of many atoms and molecules. However its applicability to partial CS has not been considered so far. In the paper [**H13**] we analyzed briefly partial cross sections for C_2H_2 molecule showing that BEB has also the potential to describe a production of certain specific ions. The detailed research on this issue is in progress.

The last problem described in [**H13**] is related to the angular resolution error in the beam attenuation methods for measuring TCS and the reliability of available low-energy experimental TCS for polar molecules. Due to the presence of long-range dipole potential ($\sim r^{-2}$), electrons are most efficiently scattered at very low angles when colliding with a polar target. The beam attenuation methods are unable to distinguish these low-angle scattered electrons from non-scattered beam because of the finite sizes of the apertures at the entrance and exit walls of the scattering chamber. This results in an underestimation of measured cross-section values, particularly in the low energy range. In work [**H13**] this problem is illustrated by comparing elastic integral cross sections obtained by an integration of the latest DCS for H_2O [76] and CH_3Cl [**P9**] with experimental TCS [83, 84, 85, 86]. Since DCS are measured in a limited angular range, the numerical integration procedure requires an extrapolation of the cross sections to small and large scattering angles (to $\theta = 0^o$ and to $\theta = 180^o$), which are difficult to be accessed experimentally. For this purpose, the extrapolation method described in [**H10**] is used. This method includes the Born correction for the dipole scattering potential (r^{-2}). The need to incorporate this correction in the theoretical description of low-energy electron scattering by polar molecules is clearly demonstrated by SMC calculations in Ref. [**P9**]. The comparision of integrated DCS with some old experimental TCS [83, 84] shows that the latter are significantly underestimated at low energies. Therefore, an accurate correction of the angular resolution error is necessary in the attaenuation-type experiments when studying polar molecules. Such attempts have been reported in more recent works [85, 86].

5.6   Summary and significance of the publication series

The knowledge of cross-sections for electron and positron scattering from atoms and molecules is essential for modeling a wide range of phenomena that are relevant in many different areas such as the plasma diagnostics in new generation of fusion reactors, the plasma etching in semiconductor technology, the studies of radiation damage in living matter and the research on the matter - antimatter interactions. Despite long and intensive works, there are only few atoms and molecules for which the full representation of electron scattering cross-sections for all partial processes can be proposed with confidence. The situation is even less optimistic for positrons since the available cross sections are very sparse. In this publication series, using semi-empirical analysis and experimental measurements I studied cross-sections in the angular and energy ranges where the available data are particularly uncertain. The goal was to proposed consistent sets of cross-sections. The additional goal was to increase our understanding of the charged particle interaction with atoms and molecules. Here I will summarize once again the most important results described in the considered publication series:

- Paper [**H1**] proves in a detailed way that "popular" Modified Effective Range Theroy (MERT) [12] formulated within the new frames [14] can be used to describe elastic scattering cross-sections in much wider energy range than its original version [13]. In particular it was shown that MERT can be used to determined cross-sections from the zero energy up to the ionization thresholds for electron scattering from helium (He), argon (Ar) and

molecular hydrogen (H_2). In addition, it was shown that the model can describe cross sections for positron collisions. Interestingly, it predicts the presence of Ramsauer - Townsend minimum in positron scattering from all four studied targets (He, Ar, H_2, CH_4) despite an absence of clear minima in total cross-sections.

- Papers [**H2**, **H3**, **H4**] report the continuation of the MERT analysis from [**H1**] for electron scattering from noble gas atoms: neon, krypton and xenon. In all these three works I showed that MERT can be used to describe cross-sections in a very wide energy ranges. In all papers I proposed consistent and compatible sets of elastic cross sections that reproduce the results of the beam attenuation (total CS), the cross-beam (differential CS) and the swarm experiments (momentum transfer CS). In [**H4**] I also summarized the MERT analysis of the scattering length for all noble gases showing that this quantity depends linearly on atomic polarizability.

- In paper [**H5**] I proposed elastic and vibrational cross-sections for electron scattering from methane (CH_4) in the energy region of the Ramsauer-Townsend minimum. The cross-sections were derived using a semi-empirical analysis (MERT and Boltzmann's transport equation) of the latest experimental data. Recommended cross sections are in very good agreement with three different types of experiments: the beam attenuation (total CS), the cross-beam (differential CS) and the swarm (momentum transfer CS).

- In paper [**H6**] I showed that the combination of MERT with the model proposed by Gribakin [56] can be used to describe (using few parameters) the scattering cross-sections for annihilation of positrons on atoms and small molecules. Moreover, in this work I propose elastic cross sections for benzene (C_6H_6) and cyclohexane (C_6H_{12}) in the low energy range, which are in line with the results of two qualitatively different experiments: the beam attenuation one [57] and annihilation one [30].

- In the paper [**H7**] for the first time the effective range theory is formulated within the frame of Bayesian statistics. In this way the model gains a more probabilistic character. Bayesian predictive analysis of the scattering length for $e^+ - H_2$ collisions showed that only two experiments [53, 54] among three the most recently published [53, 50, 54] are compatible with the scattering length defined by Mitroy and colleagues [55]. This last value should be treated as a reference point in the cross-section analysis for H_2. This finding was confirmed in the recent work [51], where the authors of [50] corrected their experimental data due to an angular resolution error. Moreover paper [**H7**] showed that MERT is able to take into account the contribution of virtual positronium formation within the frame of short-range effects parametrization. The lack of virtual positronium in theoratical approaches leads to underestimation of cross-sections below the threshold for real positronium formation as shown in the [**H7**] by DFT calculations.

- DFT calculations published in [**H8**] showed that theorretical reconstruction of "flat" part in the energy dependencies of positron scattering cross-sections (appearing just below the threshold for real positronium formation in many atoms and molecules) requires to take into account higher order terms in multipole expansion of long-range polarization potential. The addition of higher order terms compensates the lack of virtual posittronium in short-range interactions. In [**H8**] the hypothesis of the virtual positronium was stronger confirmed by showing that the mean value of the elastic cross-sections (σ) in the "flat" part for Ar and Kr are compatible with the covalent radii (r_c) of these atoms estimated from crystallographic data, if we apply a simple relation: $\sigma = \pi r_c^2$. This indirectly confirms the hypothesis of the virtual positronium formation.

- A simple model of potential: an infinite barrier + polarization ($\sim r^{-4}$) has been tested in [**H9**] for a description of elastic cross sections for positron scattering from noble gases and simple molecules (H_2, N_2, CH_4). Excellent agreement between the model and experimental data shows that the low-energy positron collisions with simple targets can be easily modeled with any empirical approach if the long-range polarization potential is included. By the way, it was shown that the "flat" part of the cross-sections scales with the size of the rigid ball (i.e. the infinite potential barrier).

- Papers [**H10**] and [**H11**] report the measurements of the differential cross sections for the polar molecule of isobutanol (C_4H_9OH) and the nonpolar molecule of pentane (C_5H_{12}). Both studies identified resonances in the elastic scattering channel. Similar resonances should be expected in a similar energy ranges in inelastic channels due to channel coupling phenomena.

- Papers [**H12**] and [**H13**] are review articles about scattering cross-sections. Both were written for the plasma science community to indicate some systematics in cross-sections that may help in constructing the reference datasets. Both papers are related to the authors' involvement in the work of the international research group [4], which main goal is to propose coherent sets of electron cross-sections for plasma-relevant targets.

The considered publication series concerns the determinations of electron and positron scattering cross-sections using semi-empirical analysis and experimental measurements. The research involves also the tests of coherence, compatibility and correctness of available datasets, the search for systematic relationships and the studies on the nature of low-energy positron interaction with the gas-phase matter. My present research activity focuses on the construction (from scratch) of an experimental system for low-energy electron and positrons scattering from atoms and molecules in the gas phase. It will be first such kind of apparatus in the Institute of Physics of Nicolaus Copernicus University. This work is currently carried out within the framework of the scientific project in which I am the principal investigator.

6 Other scientific achievements:

A Peer-reviewed publications that are not included in the publication series but written after obtaining the Ph.D. degree

Nr	Publication	IF	5-year IF
P1	**K. Fedus**, G. Boudebs, *Kerr-induced nonlinear focal shift in presence of nonlinear absorption,* J. Opt. **14**, 035205 (2012)	1.990	1.765
P2	**K. Fedus**, G. Boudebs, *Experimental techniques using 4f coherent imaging system for measuring nonlinear refraction,* Opt. Commun. **292**, 126 (2013)	1.258	1.542
P3	T. A. Oliveira, D. Manzani, E. L. Falcao-Filho, Y. Messaddeq, G. Boudebs, **K. Fedus**, C. B. Araujo, *Near-infrared nonlinearity of a multicomponent tellurium oxide glass at 800 and 1.064 nm,* Appl. Phys. B **115**, 1 (2014)	1.856	1.686
P4	F. Bianco, **K. Fedus**, F. Enrichi, R. Pierobon, M. Ghulinyan, G. Pucker, L. Pavesi, *Two-dimensional micro-Raman mapping of stress and strain distributions in strained silicon waveguides,* Semicond. Sci. Tech. **27**, 085009 (2012)	1.921	2.037
P5	A. Karbowski, **K. Fedus**, J. Patyk, Ł. Bujak, G. Karwasz, *Photoluminescence and positron annihilation lifetime studies on pellets of ZnO nanocrystals,* Nukleonika **58(1)**, 189 (2013)	0.357	0.450
P6	A. Podhorodecki, L. W. Golacki, G. Zatryb, J. Misiewicz, J. Wang, W. Jadwisienczak, **K. Fedus**, J. Wojcik, P. R. J. Wilson, P. Mascher, *Excitation mechanism ...—Do we need silicon nanoclusters?,* J. Appl. Phys. **115**, 143510-1 (2014)	2.183	2.126
P7	**K. Fedus**, *Positron annihilation in benzene and cyclohexane: a comparison between gas and liquid phase,* J. Phys. Conf. Ser. **618**, 012029-1 (2015)	-	-
P8	**K. Fedus**, G. Karwasz, Z. Idziaszek, *Positron and electron scattering on atoms and molecules–modified effective range theory revisited,* Eur. Phys. J.-Spec. Top. 222, 2335 (2013)	1.760	1.633
P9	C. Navarro, A. Sakaamini, J. Cross, L. R. Hargreaves, M. A. Khakoo, **K. Fedus**, C. Winstead, V. McKoy, *Low-energy elastic electron scattering from chloromethane, CH3Cl,* J. Phys. B: At. Mol. Phys. **48**, 195202-1 (2015)	1.833	1.681

P10	A. Sakaamini, C. Navarro, J. Cross, L. R. Hargreaves, M. A. Khakoo, **K. Fedus**, C. Winstead, V. McKoy, *Low-energy elastic electron scattering from chloroethane, C2H5Cl,* J. Phys. B: At. Mol. Phys. **48**, 205202-1 (2015)	1.833	1.681
P11	G. Karwasz, **K. Fedus**, K. Służewski, D. Stolarz, A. Krzysztofowicz, M. Gagoś, *Inside the didactics of colours - red-cabbage juice as a teaching tool,* Colour and colorimetry : multidisciplinary contributions. Vol. 9 B / ed. by Maurizio Rossi, (Santarcangelo di Romagna, Maggioli, 2013)	-	-

B Discussion of other scientific publications written after obtaining Ph.D. degree:

Excluding the publications that appeared before obtaining the Ph.D. degree and the works that are covered by the publication series described in the previous chapter, my remaining post-doctoral research activity covers two research fields. The first one is a continuation of the Ph.D. studies which mainly deals with issues from the field of experimental nonlinear optics. The other area of my research is completely different and it concerns the experimental characterization of condensed matter structural properties using the positron annihilation spectroscopy. This second field is compatible with the general subject of positron interaction with the matter undertaken after my employment at the Institute of Physics of the Nicolaus Copernicus University in Toruń.

6.1   Research in the field of nonlinear optics

My PhD thesis was devoted to the development of experimental methods for the characterization of nonlinear optical properties. The aim of the study was to develop the most sensitive research technique using the nonlinear imaging methods that allow the measurement of nonlinear refractive indices and nonlinear absorption coefficients of thin film materials. In the paper [**P1**] I proposed a theoretical model for describing results of focal shift measurements in the presence of nonlinearly absorbing material. This work was an extension of the research technique proposed in my Ph.D. thesis at [87], where we showed that the shift of focal point of converging lens induced by a non-absorbing material can be used to characterize optical properties of the latter.

The paper [**P2**] is a review of nonlinear characterization methods inside the $4f$ coherent imaging system. This work summarizes the main research topic of my Ph.D. thesis. On the other hand paper [**P3**] reports nonlinear optical coefficients of exotic multi-component glasses. The samples were prepared in the group of prof. C. de Araujo from the Federal University of Pernambuco (Brazil) and their were characterized by me during my Ph.D. studies.

The paper [**P4**] was written during my one-year postdoctoral fellowship in the group of prof. L. Pavesi from the University of Trento in Italy. It concerns the characterization of the mechanical stress distribution induced in the silicon waveguides by a thin layer of silicon nitride. The two-dimensional stress distribution was investigated using the confocal Raman spectroscopy. My scientific contribution consisted in developing, together with the author of measurements, a theoretical model for the determination of induced stresses based on experimental data, the interpretation of results and the preparation of the manuscript. This work was a continuation of studies carried out in the Pavesi group on the second harmonic gerernration from strained silicon waveguides. The results of this research were reported in Nature Materials [88].

After starting my work in February 2012 at the Institute of Physics of Nicolaus Copernicus University in Toruń, the research related with nonlinear optics became less important in my scientific activity because I undertook a new research subject connected with electron and positron

interactions with matter (gases, liquids and solid bodies). Nevertheless, research in the field of nonlinear optics has not been completely abandoned and I still maintain the cooperation with prof. G. Boudebs from the Photonics Laboratory of the University of Angers in France. My recent work (currently submitted in Optical Materials) is based on my measurements carried out during my visit (as an invited professor) in France in September 2016.

6.2 Material characterization using positron annihilation spectroscopy

Another subject undertaken by me after PhD is related with the material characterization using positron annihilation lifetime spectroscopy (PALS). This experimental technique is nowadays well recognised as a powerful tool for investigation of defects in microstructure of condensed matter. It allows for a detection of structural changes at an early stage of their formation when they could not be detected by other spectroscopic methods (including the optical microscopy, the transmission electron microscopy and the X-ray diffraction).

Paper [**P5**] reports the experimental studies on interrelationships between the X-ray diffraction patterns, the photoluminescence spectra and the positron lifetimes obtained from circular pellets composed of ZnO nanoparticles. My contribution to this work consist in coordinating all research, interpretation of results and manuscript preparation. The main objective of the study was to investigate the evolution of defects in nanocrystals as a function of the annealing temperature and their influence on photoluminescence spectra. A typical ZnO spectrum consists of a "constant" peak in the UV range and a wide and variable band (in intensity and position) in the visible range. The origin of UV emission is well explained by the near-band-edge excitonic transitions. On the other hand, the origin of visible emission is not quite clear since it is probably related to unknown defects. This hypothesis is strongly supported by the variability of visible band depending on the production method of nanocrystals . The ZnO samples studied in work [**P5**] were characterized by a broad green band with maximum at about 500nm. According to the most popular interpretation, such kind of emission should originte from zinc vacancies. However, the results from [**P5**] did not confirm this hypothesis.

Paper [**P6**] was written in collaboration with prof. A. Podhorodecki from Wroclaw University of Technology. This study was devoted to the mechanisms of excitation and emission in silicon rich silicon oxide (SRSO) doped by terbium atoms. My contribution consists of the characterization of defects evolution with silicon nanocrystals concentration using PALS method. The final results showed no lifetime dependence on the silicon concentration, indicating that the defects responsible for optical properties of studied samples are probably undetectable or insensitive to the measurement technique.

Paper [**P7**] reports the comparative study for room-temperature positron direct annihilation in gas and liquid phases of two organic molecules: benzene (C_6H_6) and cyclohexane (C_6H_{12}). The measurements of annihilation signal in the gas phase [30] indicate that C_6H_{12} has a higher (thermally averaged) annihilation cross-section than C_6H_6. This observation is also confirmed by the MERT analysis of elastic cross-sections [**P7**] in the thermal energy range. The MERT fit to the available experimental total cross-sections gives higher values of cross-sections at low energies for C_6H_{12} suggesting also greater probability of annihilation for this molecule. This result is independent on the sign of scattering length, which is estimated from experimental values of positron binding energy to both studied molecules. On the other hand, the measurements [**P7**] of the positron lifetimes in the liquid phase indicate an opposite trend, the lifetimes for liquid benzene are shorter than for cyclohexane suggesting larger annihilation cross section for this first molecule. The reason of this difference is still to be explained.

6.3   Other publications

The remaining papers [P8, P9, P10] are related to my main research topic: the electron and positron scattering on atoms and molecules in a gas-phase. However these works are not included in the considered publication series for two different reasons. Firstly, the paper [P8] is a post-conference work, which is based on the results published in [H1]. On the other hand [P9, P10] report the original experimental results of differential cross-sections (DCS) for two polar molecules, chloromethane (CH_3Cl) and chloroethane (C_2H_5Cl), in a similar manner as the articles [H10, H11]. However my contributions to both studies are less significant than in works [H10, H11]. I participated in discussions and analysis of experimental results. Both work demonstrate the characteristic features of DCS for polar molecules: electrons are most effectively scattered at low angles due to the dominant influence of the long-range dipole potential, while the short-range effects determine the shape of the angular dependence in medium and large angles. Moreover, for CH_3Cl [P9], the presence of C-Cl σ^* (3.5 eV) shape resonance, reported in other scientific publications [90, 91], was confirmed. One of the most important result in the paper [P9] is the estimated set of integral elastic cross-sections, which turned out to be significantly higher in the low energy range than the total cross sectionas measured by the attenuation methods [84, 92, 93]. This result clearly demonstrates the effect of angular resolution error on the attenuation-type measurements, which is particularly important for polar molecules (see detailed discussion in Chapter 5.5).

To best of our knowledge, the papers [P10] reports for the first time the results of DCS for chloroethane in such wide energy ($5 - 130^o$) and angular ranges ($1 - 50$ eV). We know only the measurements reported in the Ph. D. thesis by V. K. Chan [94], which were carried out in much narrower ranges. The experimental results and SMC calculations show the presence of two shape resonances for this molecule: C-Cl σ^* (2.6 eV) and C-Hσ^* (7.5 eV).

The peer-reviewed paper [P11] deals with the innovative methods of teaching about the physics of colors and it was written as part of the statutory tasks of the Division of Didactics of Physics, Nicolaus Copernicus University.

C Tabular summary of scientific achievements

A detailed bibliometric analysis is included in Appendix No. 4.

Number of scientific publications:

	before Ph.D.	after Ph.D.	total
Number of scientific publications	**16**	**26**	**42**
Publications in journals included in *Journal Citation Reports* (JCR)	15	22	**37**
Publications in journals not included in *Journal Citation Reports* (JCR)	1	2	**3**
Academic scripts	0	2	**2**

Impact factors:

Summed *impact factor* by *Journal Citation Reports*	**68.756**
Averaged *impact factor* by *Journal Citation Reports*	**1.809**
Summed *impact factor* by *Journal Citation Reports* - 5-year IF	**62.615**
Averaged *impact factor* according to *Journal Citation Reports*	**1.680**

Summed number of citations dated on 08 May 2017:

	Web of Science	SCOPUS
Number of citations	**254**	**301**
excluding self-citations	**145**	**102**
Hirsch index	**9**	**10**

Participation in national and international scientific conferences:

	before Ph.D.	after Ph.D.	total
Summed number of conferences	**6**	**13**	**19**
Oral talks (delivered personally or by co-authors)	5	8	**13**
Posters	1	5	**6**

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