



**University
of Gdańsk**

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Uniwersytetu Gdańskiego

Summary of Professional Accomplishments

Aneta Lewkowicz, PhD

„Molecular design via electron excitation energy and selected concentration effects in fluorescent matrices”

**Institute of Experimental Physics
Division of Biomaterials and Medical Physics
Wita Stwosza 53, 80-308 Gdańsk
aneta.lewkowicz@ug.edu.pl**

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General information

1. Name

Aneta Maria Lewkowicz

2. Diplomas, degrees conferred in specific areas of science or arts, including the name of the institution which conferred the degree, year of degree conferment, title of the PhD dissertation

- **PhD in Physics (with distinction) in the field of Molecular Physics:**

„Spectroscopic properties of hybrid materials doped with organic dyes.”

Faculty of Mathematics, Physics and Informatics University of Gdańsk
12 March 2015 r.

Supervisor: Prof. Dr hab. Piotr Bojarski

- **Chemical technology Engineer, specializing in fuel technology**

Faculty of Energy and Fuels, AGH University of Kraków
July 2010 r.

- **MSc in Chemistry**, specialization: analytical chemistry and forensic chemistry

Jagiellonian University in Kraków
July 2009 r.

- **Educational Management**– postgraduate studies, **1.06.2020**, Ateneum Academy in Gdansk

- **Pedagogic studies** - postgraduate studies, **26.02.2019**, Ateneum Academy in Gdansk

3. Information on employment in research institutes or faculties/departments or school of arts

- **Adjunct**

Faculty of Mathematics, Physics and Informatics
Division of Biomaterials and Medical Physics
University of Gdańsk
1 october 2016-present

4. Description of the achievements, set out in art. 219 para 1 point 2 of the Act:

a) Title of the achievement

As a "scientific achievement obtained after receiving a doctoral degree that represents a significant contribution of the author to the development of a specific scientific discipline" I indicate a series of thematically related publications under the collective title:

„Molecular design via electron excitation energy and selected concentration effects in fluorescent matrices”

b) List of the selected publication series

H1. Pierpaoli, M.; **Lewkowitz, A.**; Ficek, M.; Ruello, M. L.; Bogdanowicz, R. Preparation and Characterization of TiO₂/Carbon Nanowall Composite on a Transparent Substrate. *Photonics Letters of Poland* 2018, 10 (2), 54. <https://doi.org/10.4302/plp.v10i2.825>. 40 pkt MEiN IF=0.6

H2. **Lewkowitz, A.**; Baranowska, K.; Bojarski, P.; Józefowicz, M. Solvent Dependent Spectroscopic Properties of Fingerprint Reagent – 1,8-Diazafluoren-9-One. *Journal of Molecular Liquids* 2019, 285, 754–765. <https://doi.org/10.1016/j.molliq.2019.04.110> 100 pkt MEiN IF=6

H3. Pierpaoli, M.; **Lewkowitz, A.**; Ryciewicz, M.; Szczodrowski, K.; Ruello, M. L.; Bogdanowicz, R. Enhanced Photocatalytic Activity of Transparent Carbon Nanowall/TiO₂ Heterostructures. *Materials Letters* 2020, 262, 127155. <https://doi.org/10.1016/j.matlet.2019.127155>. 20 pkt MEiN IF=3

H4. **Lewkowitz, A.***; Bogdanowicz, R.; Bojarski, P.; Pierpaoli, M.; Gryczyński, I.; Synak, A.; Mońska, M.; Karczewski, J.; Struck-Lewicka, W.; Wawrzyniak, R.; Markuszewski, M. J. The Luminescence of 1,8-Diazafluoren-9-One/Titanium Dioxide Composite Thin Films for Optical Application. *Materials* 2020, 13 (13), 3014. <https://doi.org/10.3390/ma13133014> 140 pkt MEiN IF=3.4

H5. Zygadło, P.; **Lewkowitz, A.*** Structural-Spectroscopic Analysis of DFO/PVA Films as Potential Materials Used in Revealing Fingerprints on Non-Porous Surfaces. *Issues of Forensic Science* 2021, No. 312, 68–76. <https://doi.org/10.34836/pk.2021.312.4> 20 pkt MEiN

H6. **Lewkowitz, A.***; Kantor, M.; Zalewski, W.; Bojarski, P.; Mońska, M. Spectroscopic Evidence of Fluorescence by 1,8-Diazafluoren-9-One Aggregates—a Prospective New Ultrasensitive Method for Fingerprint Trace Detection. *Journal of Forensic Sciences* 2022, 67 (4), 1468–1475. <https://doi.org/10.1111/1556-4029.15039>. 70 pkt MEiN IF=1.6

H7. Pierpaoli, M.*; **Lewkowicz, A.***; Dec, B.; Nadolska, M.; Bogdanowicz, R. Impedimetric Sensing of α -Amino Acids Driven by Micro-Patterned 1,8-Diazafluoren-9-One into Titania- Boron- Doped Maze-like Nanocarbons. *Sensors and Actuators B: Chemical* 2022, 371, 132459. <https://doi.org/10.1016/j.snb.2022.132459>. 200 pkt MEiN IF=8.4

H8. **Lewkowicz, A.***; Pierpaoli, M.; Walczewska-Szewc, K.; Czarnomska, M.; Bojarski, P.; Bogdanowicz, R.; Pogorzelski, S.; Kułak, L.; Karczewski, J. Nonconventional 1,8-Diazafluoren-9-One Aggregates for Green Light Enhancement in Hybrid Biocompatible Media. *Materials* 2022, 15 (14), 5012. <https://doi.org/10.3390/ma15145012>. 140 pkt MEiN IF=3.4

H9. Miotke-Wasilczyk, M.; Kwela, J.; **Lewkowicz, A.**; Józefowicz, M. Insight into the Release Mechanisms of Diflunisal and Salicylic Acid from Poly (Vinyl Alcohol). The Role of Hydrogen Bonding Interactions. *Spectrochimica Acta. Part A, Molecular and Biomolecular Spectroscopy* 2023, 284, 121802. <https://doi.org/10.1016/j.saa.2022.121802>. 140 pkt MEiN IF=4.4

H10. Walczewska-Szewc, K.; Rydzewski, J.; **Lewkowicz, A.** Inhibition-Mediated Changes in Prolyl Oligopeptidase Dynamics Possibly Related to α -Synuclein Aggregation. *Physical Chemistry Chemical Physics* 2022, 24 (7), 4366–4373. <https://doi.org/10.1039/D1CP05238A>. 100 pkt MEiN IF=3.3

H11. Czarnomska, M.; **Lewkowicz, A.***; Pierpaoli, M.; Gruszczyńska, E.; Kasprzak, M.; Gryczyński, Z.; Bojarski, P.; Steinborn, S.; Woźniewski, K. Analysis of Friction Ridge Evidence for Trace Amounts of Paracetamol in Various Pharmaceutical Industries by Raman Spectroscopy. *Journal of Forensic Sciences* 2024;69:437–447. <https://doi.org/10.1111/1556-4029.15451>. 70 pkt MEiN IF=1.6

H12. **Lewkowicz, A.***; Walczewska-Szewc, K.*; Czarnomska, M.; Gruszczyńska, E.; Pierpaoli, M.; Bogdanowicz, R.; Gryczyński, Z. Molecular Design Using Selected Concentration Effects in Optically Activated Fluorescent Matrices. *International Journal of Molecular Sciences*, 2024, 25, 4804-4817. <https://doi.org/10.3390/ijms25094804> 140 pkt MEiN IF=5.6

c) Other post-doctoral scientific achievements not included in the habilitation publication series:

P1. Patent Application P.443382 Sposób wizualizacji śladów daktyloskopijnych na podłożu chłonnym oraz roztwór końcowy do wizualizacji śladów daktyloskopijnych na podłożu chłonnym (positive opinion- State of the Art Report September 2023, further procedure 2023/2024)

T1. Nadolska, M.; Szkoda, M.; Trzciniński, K.; Ryl, J.; **Lewkowicz, A.**; Sadowska, K.; Smalc-Koziorowska, J.; Prześniak-Welenc, M. New Light on the Photocatalytic Performance of NH₄V₄O₁₀ and Its Composite with RGO. *Scientific Reports* 2023, 13 (1), 3946. <https://doi.org/10.1038/s41598-023-31130-9>.

T2. Kunuku, S.; Ficek, M.; Wieloszyńska, A.; Tamulewicz-Szwajkowska, M.; Gajewski, K.; Sawczak, M.; **Lewkowicz, A.**; Ryl, J.; Gotszalk, T.; Bogdanowicz, R. Influence of B/N Co-

Doping on Electrical and Photoluminescence Properties of CVD Grown Homoepitaxial Diamond Films. 2021, 33 (12), 125603–125603. <https://doi.org/10.1088/1361-6528/ac4130>.

T3. Pierpaoli, M.; Jakóbczyk, P.; Dec, B.; Giosuè, C.; Czerwińska, N.; **Lewkowicz, A.**; Ruello, M. L.; Bogdanowicz, R. A Novel Hierarchically-Porous Diamondized Polyacrylonitrile Sponge-like Electrodes for Acetaminophen Electrochemical Detection. *Electrochimica Acta* 2022, 430, 141083. <https://doi.org/10.1016/j.electacta.2022.141083>.

T4. Kunuku, S.; Ficek, M.; Sengottuvel, S.; Ryl, J.; Mrózek, M.; **Lewkowicz, A.**; Wojciechowski, A.; Bogdanowicz, R. Fabrication of High-Density Nitrogen-Vacancy (NV) Center-Enriched Diamond Particles through Methyl Trityl Amine (C₂₀H₁₉N) Seeding. *Diamond and Related Materials* 2024, 142, 110860. <https://doi.org/10.1016/j.diamond.2024.110860>.

T5. **Lewkowicz, A.** Praca Projektowa Jako Praktyczna Forma Edukacji Służąca Angażowaniu Studentów W proces Uczenia Się. In *Educatio iuris- ars boni et aequi*; Balwicka-Szczyrba, M., Zajadło, J., Eds.; Wydawnictwo Uniwersytetu Gdańskiego: Gdańsk, 2023.

Statements from all co-authors of publications confirming their individual contributions to the scientific achievements are included in Appendix 5.

d) Discussion of the scientific goal of the above work, the results and their possible application

This self-reference presents a detailed description of the scientific objective and theoretical basis of the research conducted in the field of physics. However, the interdisciplinarity resulting from the application of fluorescence spectroscopy to forensic science research is one of the most significant achievements of the presented research. Forensic science, which involves the detection and analysis of traces that can be used as evidence, is crucial to law enforcement and is a constantly evolving scientific field. The motivation for the research presented was the improvement of existing procedures and the creation of new ones that could serve the development of forensic science. The results of this work were presented in the form of a scientific patent, which focused on the use of the fluorescence phenomena to reveal fingerprint traces. It will be the subject of further discussion in the remainder of this paper. The combination of scientific disciplines is a fundamental and indispensable part of the dynamic development and application of science in everyday life, and it is this element of the work that I would like to highlight as one of the most important in my habilitation process.

4.1 Introduction

Molecular physics represents a fundamental basis for advancement in a number of fields, including medicine, forensic science, pharmacy, and industrial research. It enables the development of innovative technologies, materials, and drugs. My research focuses on the obtaining new and the improvement of existing optically active materials with various spectroscopic properties at the molecular level, while maintaining aspects of key importance to these sectors, such as safety in the manufacturing and application processes of new materials.

In molecular design, I am particularly interested in the phenomenon of aggregation. While the historical research on aggregation processes is extensive [1-16], the application of such phenomena in molecular design, presented in this self-reference, is a narrative about the development of methods for obtaining and interpreting aggregation within the context of

molecular physics. It is crucial to comprehend the implications of employing a specific representation of molecule concentrations, including the capacity to generate novel structural forms while regulating the spectroscopic properties of modeled optically active materials. This understanding is essential to the successful utilization of these materials. I propose a novel approach to the potential for controlling aggregation processes to obtain the corresponding spectroscopic and photophysical properties of materials.

I presented an innovative approach to molecular spectroscopy that fully utilizes photophysical characteristics, in contrast to the current approach in molecular design, which is mainly based on molecular structure analysis to obtain materials with the required properties [17-20]. While molecular structure is crucial, consideration of aggregation processes is of broader importance for correct spectroscopic and physicochemical interpretation [21-22]. The possibility of occurrence of the aggregation-induced emission (AIE) phenomenon that I presented represents a novel approach for the molecule 1,8-diazafluoren-9-one (DFO) and occurs in various matrices. This phenomenon is known previously for other molecules and matrices [23-24]. In the case of my research, methodologies for obtaining various materials using this physical phenomenon have been extended. I believe that the approach I presented is a significant contribution to the field of spectroscopic methodology, particularly in the design of AIEs for DFOs in select media. This methodology has the potential to be of significant value in the context of the development of novel fluorescent and electrochemical probes.

It is also worth noting that the differences in spectroscopic properties between the DFO monomer and its aggregates can be attributed to changes occurring at the molecular level, as well as during the aggregate formation stage. The interpretation of the aggregation phenomenon, which has often been overlooked in favor of the molecular structure, within the framework of the publications I have presented is essential, as the influence of the aggregate-monomer interaction is important when describing the characteristics of the changes occurring in the surrounding molecular environment. The objective of the research presented is to understand the differences in physical, photophysical, and spectroscopic properties between the state of a single molecule and its aggregated form. The influence of the aggregation phenomenon on the properties of materials is also addressed, as well as the development of a methodology for optimization in terms of the required application properties.

In papers [H1-H12] and [P1], I presented molecular physics analyses targeting the design of molecular probes and the phenomenon of sensibilization to serve the identification of a specific group of alpha amino acids in different environments/matrices. The selective intermolecular interaction between the sensoribilizer attached to the designed matrices and the target amino acid induces increased excitation energy transfer in the electron band, which allows for the determination of spectral features through the application of spectroscopic mapping techniques, including stationary and time-resolved. The calculations presented in the paper [H12] suggest a mechanism based on the possibility of an “in situ” chemical reaction occurring as a result of controlled aggregation processes, accompanied by local charge redistribution, affecting the lowering of the potential energy barrier in a specific part of the newly formed cyclodimer—an aggregate previously unknown in the literature from the point of view of controlling the aggregation process. The model laboratory procedure I have introduced uses various media as matrices for the fluorophore. The spectroscopic activity of these materials is controlled by analyzing the mechanisms of concentration quenching of photoluminescence. As part of the present research, the following activities have been carried out:

- I have developed a characterization of the concentration quenching of photoluminescence conditioned by the presence of dimers and higher-order aggregates for the molecule 1,8-diazafluoren-9-one (DFO) [H4-H6, H8, H12].

- I have developed a characterization of spectroscopic properties that indicate possible excitation energy transfer pathways for the molecule 1,8-diazafluoren-9-one and structures formed in rigid matrices due to the phenomenon of controlled aggregation [H4, H6, H8].

- I proposed a new method to synthesize the molecule - DAK DFO based on the phenomenon of aggregation [H12].

- I pointed out the possibility of the coexistence of various luminescence centers, whose deactivation of excited states is based not only on radiative processes, but the significant influence of non-radiative excitation energy transfer processes [H4, H8, H12].

- I presented the possibility of the occurrence of non-radiative energy transfer from excited monomers to nonluminal dimers-a phenomenon observed for DFO in solution, but also for TiO₂ matrices [H4, H6].

- I presented potential applications of aggregation phenomena in solutions and rigid systems to real systems and attempted to implement the experimental results obtained. [H6, H12, P1].

- I described the physical and chemical procedures within molecular design that affect the environment and molecule concentrations, and thus the selected photoluminescence properties of the analyzed systems [H1-H4, H7-H10].

- I developed procedures for the structural analysis of novel materials using Raman spectroscopy for molecular design [H1, H3, H9, H11].

In referring to the above point, I have presented a coherent photophysical characterization of concentration phenomena, including the issues of concentration quenching and fluorescence quenching by foreign absorbing substances present in real systems.

The presented series of publications [H4-H6, H8, H12] demonstrates the potential for controlling the deactivation of the energy of excited states by selecting a dye, the so-called luminescent probe, and regulating the components of the matrix, which was obtained "in situ" during the aggregation of the dye. The excitation energy can be consumed in various ways, such as heat loss, extensive emission processes, or as a result of photochemical reactions. In the cases considered, particular attention was given to radiative deactivation processes and the potential for a photochemical cyclodimerization reaction of the analyzed dye in a given environment. It is also essential to consider energy deactivation processes in a non-radiative manner. This was possible to observe at the molecular level during the concentration quenching process in the designed materials. The effect of substance concentration on luminescence has been described in numerous works for many years (1-32). However, the approach within the framework of my postdoctoral work takes into account the particular possibility of chemical activity of the molecule under analysis, while controlling the concentration aggregation conditions.

- Furthermore, I presented the mechanism of the solvatochromic effect for the DFO [H2] dye, which is interesting from the perspective of its potential applications in forensic science or medicine. I investigated its solvatochromic properties and presented its photophysical properties with particular emphasis on its molecular characteristics. This has led to further potential applications of this molecule in the molecular design of matrices as marker materials for alpha

amino acids, which could indicate the presence of cancer or a sweat-fat substance. This could also map the arrangement of fingerprints in a dactyloscopic trace.

In my research, I presented the key role of intermolecular interactions and the development of methodologies for their control, with special emphasis on concentration effects such as aggregation or the possibility of excitation energy transfer in the monomer-aggregate system. The result of molecular spectroscopy research is the proposed method based on the analysis of absorption and fluorescence spectra in stationary and time-resolved modes, and the observation of changes in photophysical properties characteristic of interacting fluorescent centers in the UV/VIS electromagnetic radiation range. The method was designed to account for the effects observed in the real system (rigid matrices) at different concentrations, timescales (stationary and picosecond), and chemical factors. This approach allows for a quantitative description of the processes occurring in the system, including the influence of competing reactions that may occur due to the complex nature of the real system.

The presented research results enabled the utilization of the spectroscopic and photophysical properties of the DFO molecule to develop a patent procedure [P1].

The subject of the invention is a method of visualizing dactyloscopic traces on an absorbent substrate (plain paper and thermal paper) using a non-toxic final solution based on aggregates of 1,8-diazafluoren-9-one in a polyvinylpyrrolidone polymer and with the addition of Au/Ag core-shell nanoparticles. These nanoparticles increase the fluorescence of the revealed dactyloscopic trace, enabling dactyloscopic analysis. It is noteworthy that the utilization of this methodology enables the visualization of the dactyloscopic trace outside of the forensic laboratory, without the necessity of a fume hood. Furthermore, the toxicity of the reagents utilized has been significantly reduced. This represents a substantial contribution to the development of methods and procedures employed at the scene. This innovation represents a significant advance in the field of forensic science. By controlling aggregation processes and optimizing the medium/environment for fluorescent dyes, it is now possible to visualize forensic traces quickly and with significantly reduced toxicity compared to previously used methods.

In conclusion, stationary absorption and emission spectroscopy, in conjunction with time-resolved emission studies, were employed to validate the spectroscopic characteristics of novel molecular structures (fluorophores) under targeted aggregation conditions.

4.2 Solvatochromism as a physical phenomenon that allows observation of changes in photophysical properties during molecular design.

The main objective of this study was to present the so far unknown literature photophysical characteristics of the molecule 1,8-diazafluoren-9-one (DFO) in different environments and two states of matter: gaseous and liquid. The interest in changing the photophysical characteristics of DFO as a result of different solvent polarity, i.e. solvatochromic sensitivity, arose from previous literature reports on a type of this compound - the fluorenone group of aromatic ketones [33-38]. DFO is an aromatic ketone, a carbonyl compound in which the -CO group is near the aromatic ring configuration.

The paper [H2] focuses on the changes in spectroscopic properties after a molecule has acquired an excited state due to the absorption of a quantum of electromagnetic radiation from the

UV/VIS light range. A quantum of light from this electromagnetic region has sufficient energy to move an electron to a higher energy level, where the most commonly considered electron excitation in aromatic ketones concerns $n \rightarrow \pi$ or $\pi \rightarrow \pi^*$ transitions. The change in the energy level of the molecule (electron transition) is associated with the absorption and emission of a photon with an energy equal to the difference in energy levels of the ground and excited states of 1,8-diazafluorene-9-one. The excited electrons return to the ground state, which is the state with the lowest possible energy, spontaneously. The energy can be transferred to the environment, i.e. to the solvents to be analyzed. It is very important to present the electron transitions in a complete spectroscopic manner, i.e. taking into account all physical factors, including the analysis of the dipole moments of the DFO molecule in the ground state and excited states.

Among my original achievements is the photophysical analysis of 1,8-diazafluoren-9-one, not yet described in the literature, at the same time a first step towards application and the planning of further research activities on the detection of α -amino acid markers (DFO in the form of both luminescent and electrochemical probes).

The preparation of samples in the form of DFO solutions in solvents of different polarity and the measurement of absorption and emission spectra, followed by their photophysical analysis, have been presented in papers [H2 and H6]. A full characterization of the processes following electron excitation is presented, which is an important contribution to further studies performed with this molecule in other environments including rigid matrices.

The use of DFO as a selective probe for the identification/discovery of α -amino acids is possible upon prior knowledge of the influence of the local environment of the fluorophore of interest (DFO). The characterization started from the baseline, i.e. with the presentation of the energy level structure of the substance in systems without the influence of the environment, i.e. in the gaseous state. Subsequently, the influence of the surroundings of the DFO molecule on its absorption and fluorescence spectrum was investigated, considering the spectral range (position), intensity, and optical contour (shape) of the band.

I have described for the first time the solvatochromic dependence of this molecule, further suggesting the possibility of using it as a probe that is sensitive to changes in the polarity of the local environment.

An answer to the next question: can a molecule, a dye, affect the local arrangement of solvent molecules? It was presented in the publication [H2]. I carried out a comparison with my research team between the original molecule (Fluoren-9-one) and its derivative (1,8-diazafluoren-9-one) which had an additional two nitrogen atoms incorporated into the aromatic ring. The indicated structural difference significantly affected the photophysical properties and local dependence of the molecule - Figure 1 and Figure 2.

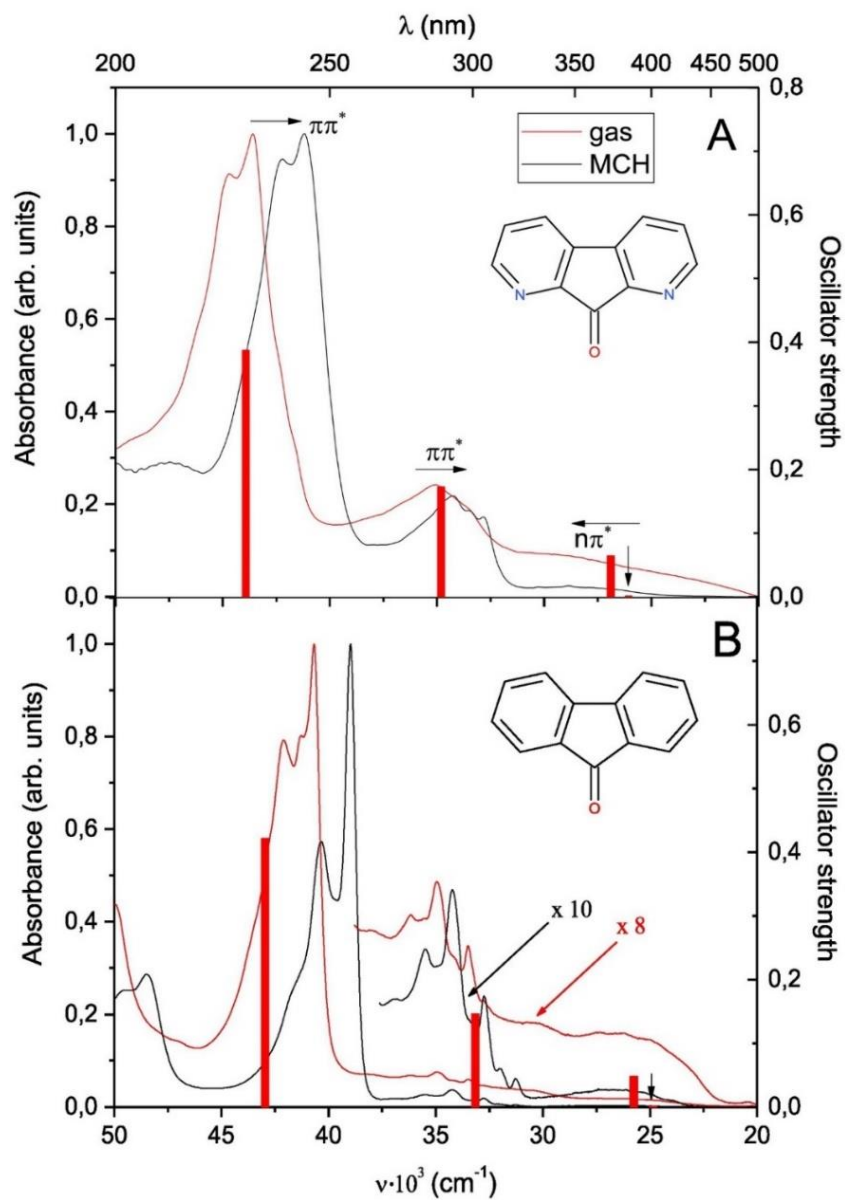


Figure 1. Absorption spectrum of 1,8-diazafluoren-9-one and fluoren-9-one [H2].

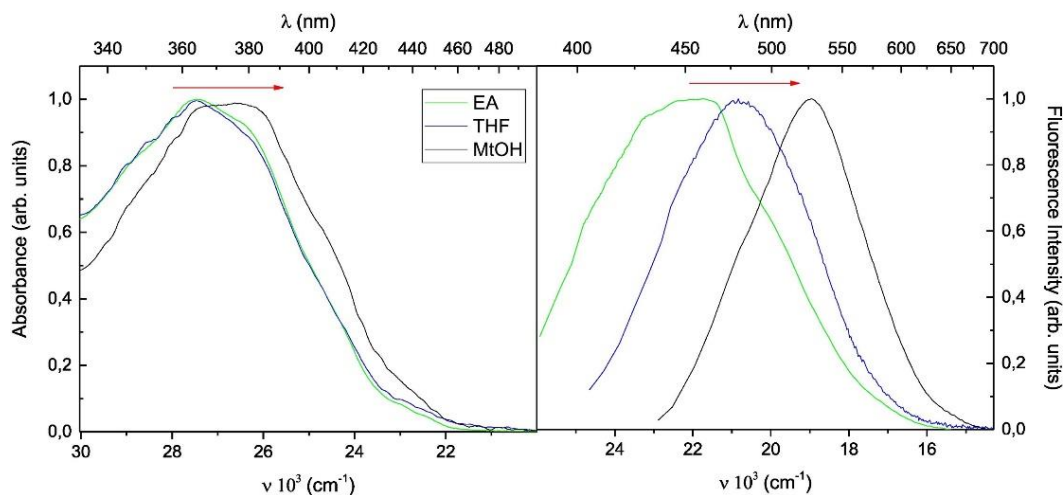


Figure 2. Absorption and fluorescence spectra of DFO in solvents of different polarity [H2].

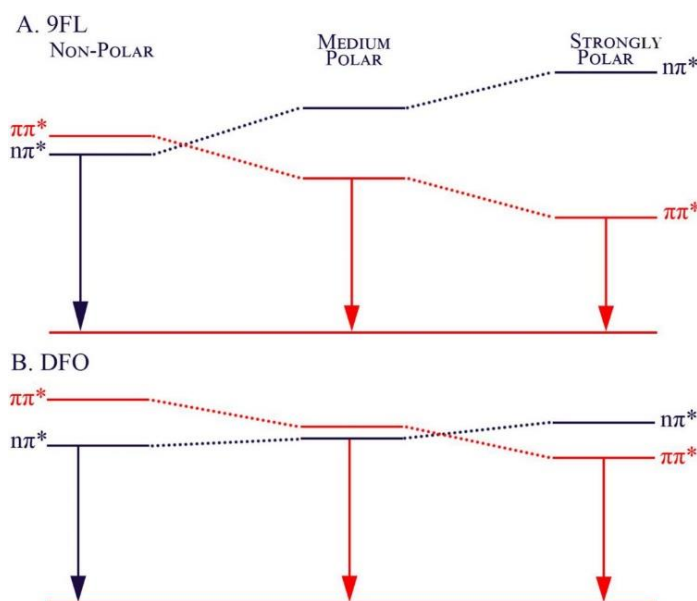


Figure 3. Structure of the electron energy levels for the DFO molecule and fluoren-9-one [H2].

A characterization of the influence of the local environment on the photophysical properties of the DFO molecule was obtained. Intermolecular interactions between the DFO molecule and solvents of different polarity are important, especially where hydrogen bridges are formed, so different types of electron states may be involved in energy transfer; in polar environments, DFO is active in the $\pi \rightarrow \pi^*$ states - Figure 3. Interactions between the DFO molecule and a protic solvent are characterized by changes in the dipole moments of the DFO molecule in the excited state. **At this stage of my research work, I have acquired one of the most important insights into the DFO molecule, namely I have confirmed the existence of interactions between the environment and DFO. Controlling these interactions is a very important step in the design of optically active materials using organic dyes.** Observation of the position and shape of the absorption spectrum in non-polar and polar environments gives information on the influence of the local environment; moreover, the intensity of the absorption and fluorescence spectrum, as well as the direction of change towards the long-wave direction, provides information on the type of electron transition - Figure 2.

I confirmed the solvatochromic sensitivity of the DFO molecule by determining photophysical parameters that describe the change in the position of the absorption band maximum due to changes in the molecule's environment in the form of a change in solvent polarity:

- absorption band maximum in the gaseous state (inert gas environment)
- dipole moment in the ground and excited states for a DFO molecule
- Stokes shift
- analysis of the dielectric permeabilities for the local environment of the DFO molecule.

The influence of the local surroundings was evidenced by the obtained Stokes shift for the DFO molecule in solvents of different polarities. The observed increase of the dipole moment in the excited state for the DFO molecule is explained by the polarization of the electron clouds of the surrounding solvent molecules, also considering the orientation polarization. **The largest Stokes shift was observed for the most protic solvents, where, however, a longer excited state lifetime was not confirmed as for the primary fluorene-9-one molecule. This finding is very important, as it suggests the formation of new forms, in the excited state, which influence the shortening of excited state lifetimes. DFO exhibits solvatochromic sensitivity, which can be significantly controlled when designing materials with the required spectroscopic properties.**

4.3 Optically active matrices - synthesis and structural-spectroscopic characterization

The area of my photophysical interest is to make a complete spectroscopic representation of a DFO molecule. It is known that this is significantly influenced by the local environment, so a study of the optimal environment for the DFO molecule was initiated.

The first research was aimed at obtaining matrices dedicated to the DFO dye. From an experimental physicist's point of view, we can use the categorical statement: "A newly photophysical characterized molecule should be studied in a known environment". The rigid matrices obtained by my formulation are one such material. Within the framework of the presented series of publications, I have presented methods for the synthesis and procedures for the structural characterization of the obtained matrices, later proposed for further spectroscopic activities [**H1**, **H3**].

The synthesis of novel carbon nanostructures was a key point to increase the application area of currently known titanium dioxide thin films. I described a transparent heterostructured matrix by designing boron-doped carbon nanowires (CNWs) (B-CNWs) on quartz followed by simple sol-gel deposition of TiO₂ [**H1**, **H3**]. The resulting anatase titanium dioxide was uniformly deposited on the carbon nanotube layer. The underlying carbon nanowall layer played a dual role in the heterostructure: it affects the crystallinity of TiO₂ and promotes the separation of photo-excited electrons by increasing the number of contact points between the two layers. Together with the research team, I obtained an original effect of combining B-CNWs with TiO₂, which can enhance the separation of photogenerated electron-hole charges, due to the specific structure of CNWs resembling a labyrinth-figure 4 and 5.

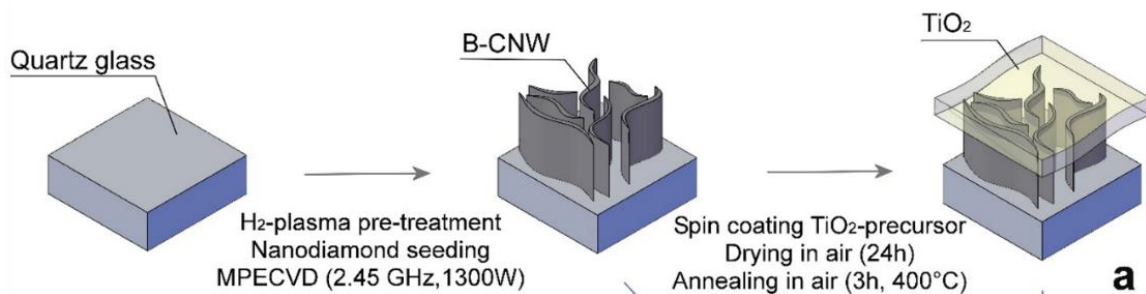


Figure 4. Structures of TiO_2 and TiO_2/CNWs thin films.

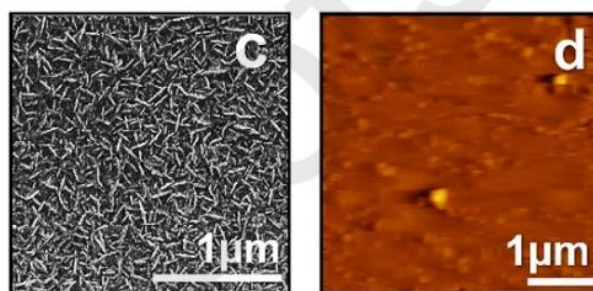


Figure 5. Images of the morphology and topography of TiO_2/CNWs thin films [H3].

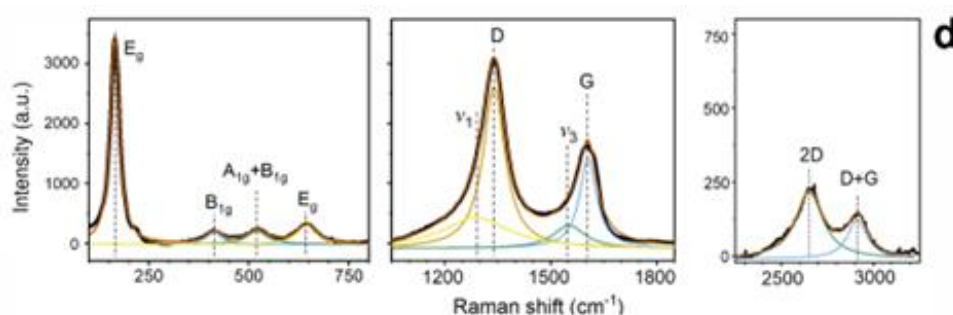


Figure 6. Raman scattering spectra for TiO_2 and TiO_2/CNWs [H3].

In the paper [H3], I used the possibility of Raman scattering measurements for titanium dioxide and carbon. **The work shows the use of analysis of excited oscillatory levels and the observation of physical processes with a change in photon energy after an oscillatory transition, without an electron transition occurring.** To confirm the quality of the structures of the obtained matrices, Raman spectra are presented in Figure 6.

A well-resolved Raman peak of TiO_2 is observed at 157 cm^{-1} for TiO_2 and at about 163 cm^{-1} for $\text{TiO}_2/\text{B-CNWs}$. $\text{TiO}_2/\text{B-CNWs}$, which is attributed to the main anatase vibrational mode followed by peaks at $\sim 413\text{ cm}^{-1}$, 526 cm^{-1} , and 645 cm^{-1} . The other two main bands at $\sim 1560\text{ cm}^{-1}$ and $\sim 1340\text{ cm}^{-1}$ are attributed to the G and D bands of the carbon nanolayers [39].

Finally, I proposed optically active rigid matrices/systems for further studies due to their high viscosity, which prevents secondary reactions and diffusion of primary products in the system. We fully control the obtained 'in situ' molecules, and new chemical structures that are used as luminescent probes.

Further proposed optically active matrices for the 1,8-diazafluoren-9-one molecule are PVA polymer films, and high viscosity media (matrices) using high molecular weight PVP polymers applied to absorbent surfaces. The work used effective control of the polymerization process during the molecular design of solid matrices as transparent media for the dye under study. In the simplest terms, polymerization is the assembly of individual units of a substance, so-called 'mers', into larger, chain-like, cross-linked structures. In the case of the research presented here, the monomer is a single atom (T, O, H) [**H1**, **H2**, **H7**, **H8**], which forms heteropolymers, i.e., chains formed by atoms of two different elements alternately by alternation. For these types of polymers, we are dealing with the dependence of the actual crosslinking energy of the macromolecule on the mode and type of positioning of the atoms in the network, so strong polarizing effects may occur. Another group of polymers studied, were organic polymers in which the mer is a PVA or PVP molecule [**H5**, **H12**, **P1**]. In the polymerizations I optimized, linear (strand shape) or globular (network with 'meshes') polymers were obtained. The dye was placed 'in situ' during the polymerization reaction. In the case of the DFO molecule, the material obtained was to have the best possible reactivity towards α -amino acids-DFO for use as a fluorescent probe. DFO is a molecule with a low fluorescence quantum yield [**H2**], which when in contact with α -amino acids is selective giving a product with a high fluorescence quantum yield - Figure 7, which was investigated by me in several papers [**H5**, **H7**, **H12**, **P1**]. The research started with a simple model medium that could be a promising matrix for DFO, this is polyvinyl alcohol (PVA). PVA is an odorless, colorless, and non-toxic polymer. Its strong hygroscopic properties and additional chemical strengths, namely biocompatibility, and biodegradability, have been exploited [40-41], allowing DFOs to be reactive with α -amino acids outside the environment and migrate inwards, and to be able to work with these materials outside the laboratory. The proposed polymers may have applications in forensic procedures, for revealing and securing forensic traces in the form of dactyloscopic traces containing α -amino acids. They are highly competitive with current procedures, where highly toxic reagents are used, including methanol - Figure 8.

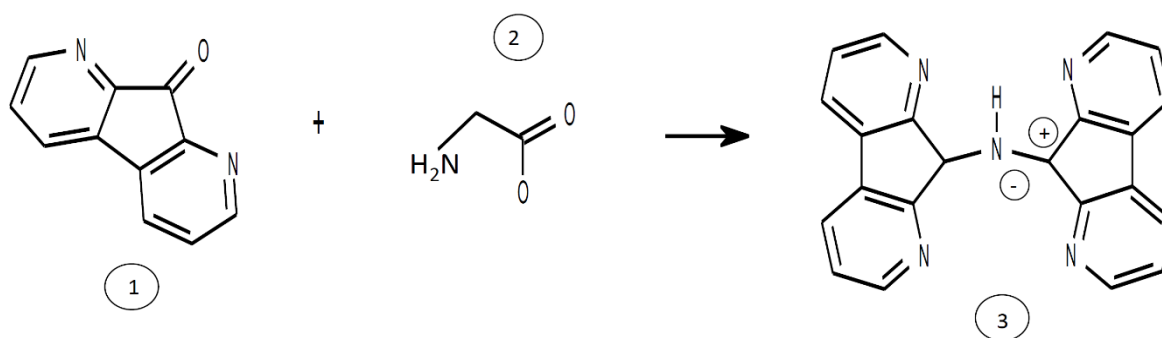


Figure 7. DFO reaction with glycine [H5].

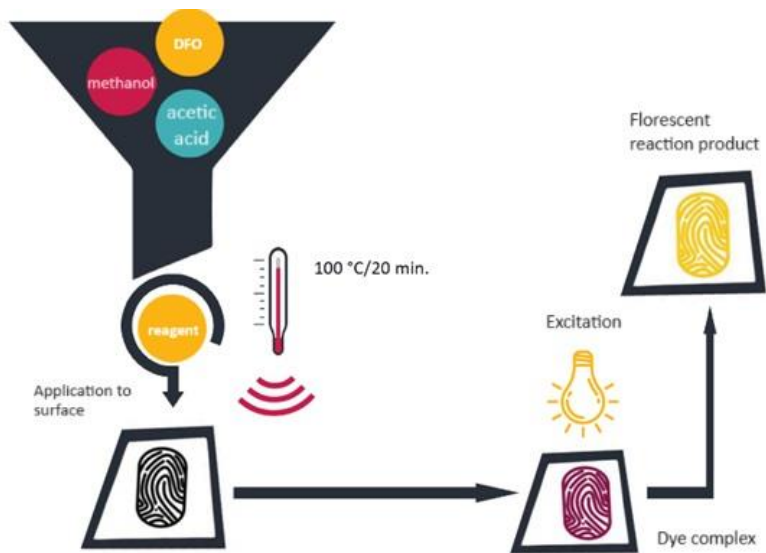


Figure 8. Current procedure for revealing dactyloscopic traces on absorbent (porous) surfaces [H5].

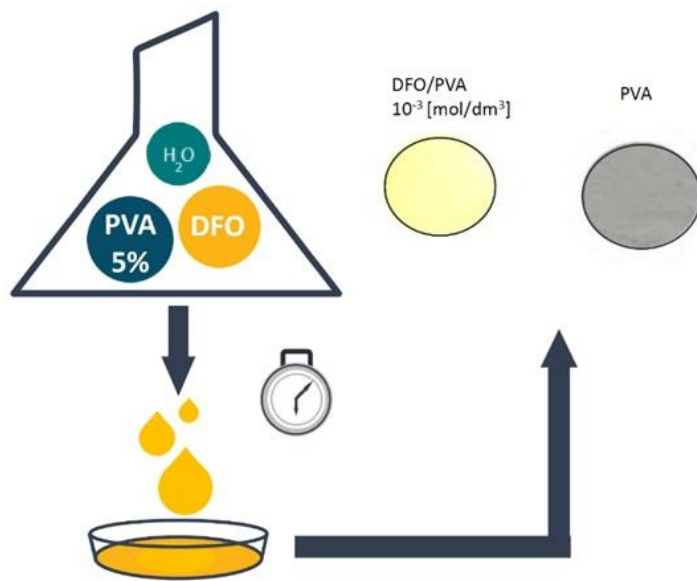


Figure 9. A new procedure for obtaining hydrogel films with high absorption to sweat-fat substance [H5].

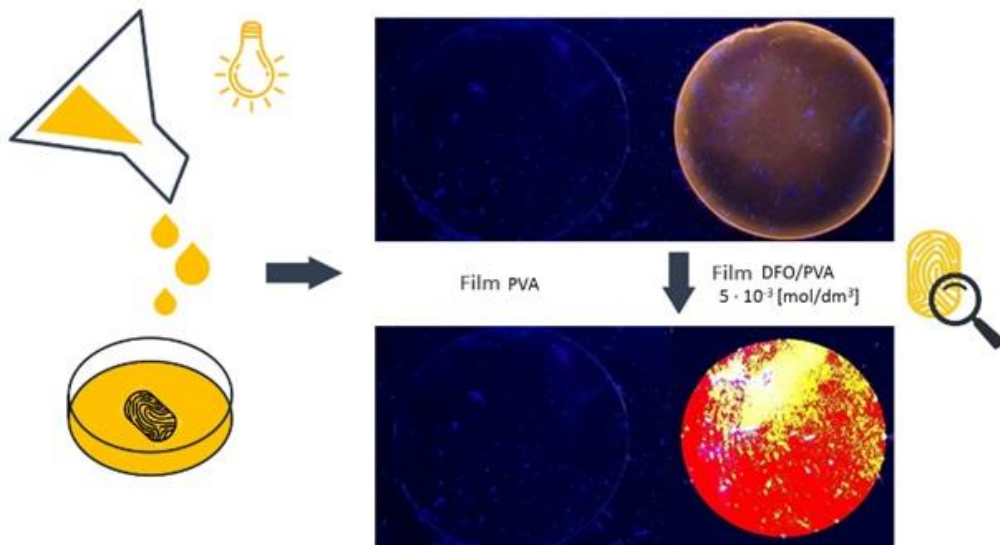


Figure 10. Procedure for revealing dactyloscopic traces on a non-absorbent surface [H5].

The resulting DFO/PVA film materials appeared to be reactive towards glycine, a representative of the α -amino acids used in the author's experiment - Figures 9 and 10. For the first time, I suggested that it is possible to use lower concentrations of DFO to reveal α -amino acids present in sweat-fat substances. I provided evidence for the presence of fluorescent aggregates, which also show the possibility of revealing dactyloscopic traces. I confirmed the imaging/visualization of these fingerprints on glass by the transfer of electron excitation energy from the excited DFO monomers to the DFO aggregates (an excitation wavelength of 380 [nm] characteristic of the excitation of DFO monomers was used, and emission characteristic of the aggregates was observed) [H5].

Studies in other rigid matrices in the form of titanium dioxide and titanium dioxide with carbon nanowires also confirmed the presence of fluorescent DFO aggregates [H7, H8].

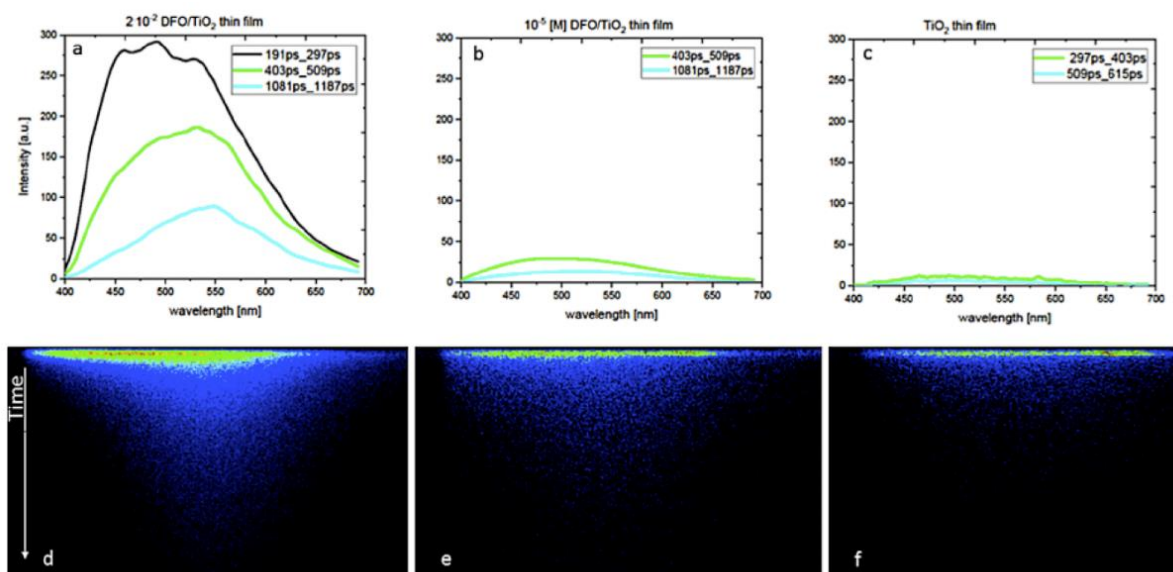


Figure 11. Fluorescence time-resolved spectra for different concentrations of DFO: (a) 2×10^{-2} [M], (b) 10^{-3} [M] in titanium dioxide matrix and (c) titanium dioxide thin films [H7].

The original contribution during the development of these results consisted mainly in the independent synthesis of all materials, optimization of the environment for 1,8-diazafluoren-9-one to fully control the photophysical properties, newly formed and discovered fluorescent DFO aggregates - Figure 11. These studies were a crucial step for further application activities using the DFO molecule. I obtained a proprietary procedure for revealing dactyloscopic traces on so-called 'difficult' surfaces, i.e., on regular and thermal paper. I have developed a Patent, which has been filed with the National Patent Office [P1], and in further steps, the results of this research have been published [H12].

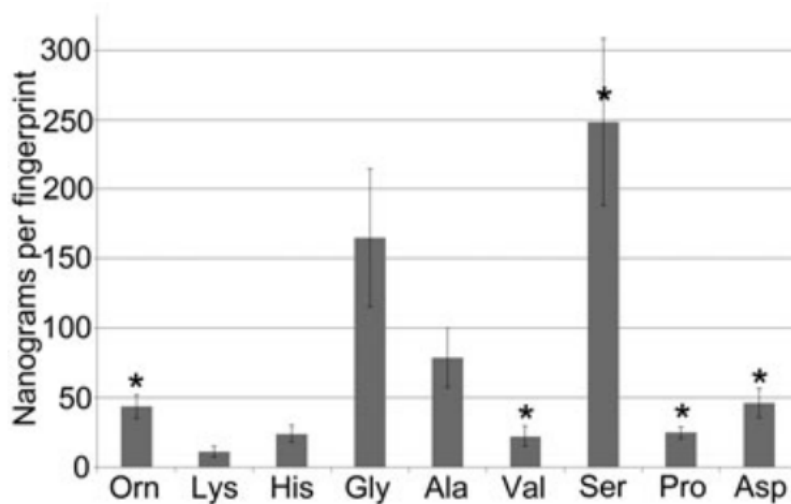


Figure 12. Alpha-amino acids in sweat-fat substance [35].

During the molecular design of the best arrangement for the DFO relative to the alpha-amino acids present in the sweat-fat substance - Figure 12 (which forms the fingerprint on the paper), I took into account the presence of leuco-dyes present in the thermal paper, so the local environment of the DFO included the PVP polymer, whose role is shown in Figure 13.

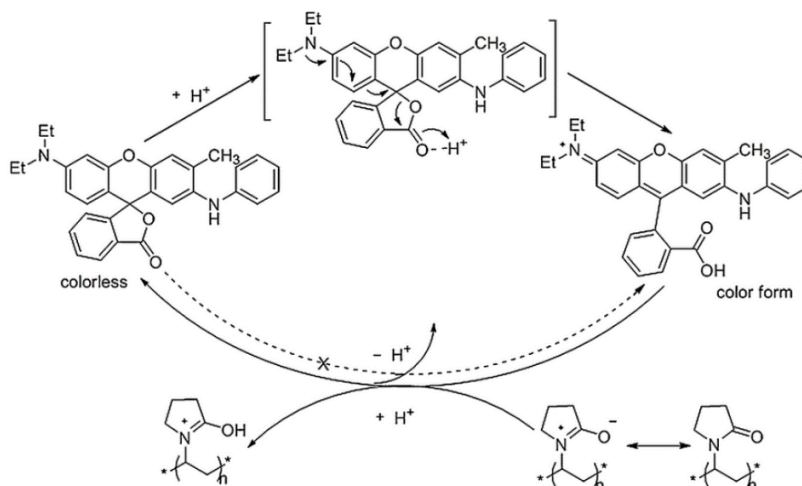


Figure 13. Black staining reaction and blocking of this process due to the presence of the PVP polymer [42].

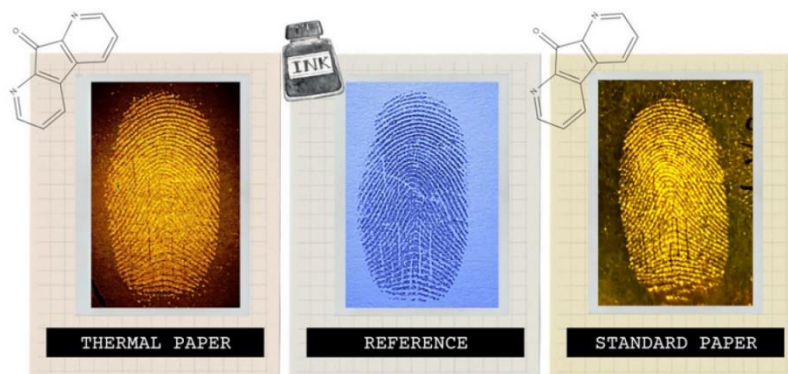


Figure 14. Visualization of fingerprint on regular and thermal paper using the original procedure [P1].

The spectroscopic effect shown in the figures was enhanced by the participation in the reaction not only of DFO monomers, forming DFO complexes with α -amino acids with high fluorescence quantum yields but also by the presence of DAK DFO dimers, which show fluorescence due to the resonant transfer of excitation energy from the dimers - Figure 14. We must not forget the presence of higher-order DFO fluorescent aggregates, this was also confirmed by the studies contained in the work [H7, H8, H5, H12]. The presence of several fluorescent centers makes it possible to obtain an enhancement effect of the fluorescence phenomenon and the possibility to use several excitation wavelengths in such an application for the disclosure of dactyloscopic traces, as developed in the patent application and publication [P1, H12].

In further molecular work on DFO, novel electrode materials have been designed as electrochemical sensors for the determination of alpha amino acids, drugs, and prohibited substances. Reliable diagnostic procedures and devices are needed not only in forensics but also in pharmacology. Therefore, the use of the DFO molecule in real-time sensory devices has been proposed. Demonstrated, a highly evolving group of chemical sensors are electrochemical sensors. The research proposed novel diagnostic electrode materials - Figures 15 and 16 [H7]. Electrochemical analysis has identified the determinants of the electrical properties of environmentally friendly electrodes and their use in the identification of alpha-amino acids and specific groups of drugs or banned substances. Measurement of the electrical signal is the basis of the proposed sensor platforms for the detection of α -amino acids and paracetamol [H7, T3]. The performed structural-spectroscopic characterization of materials in the form of boron-doped diamond (BDD) thin films has great potential in electrical and electrochemical sensors [H7].

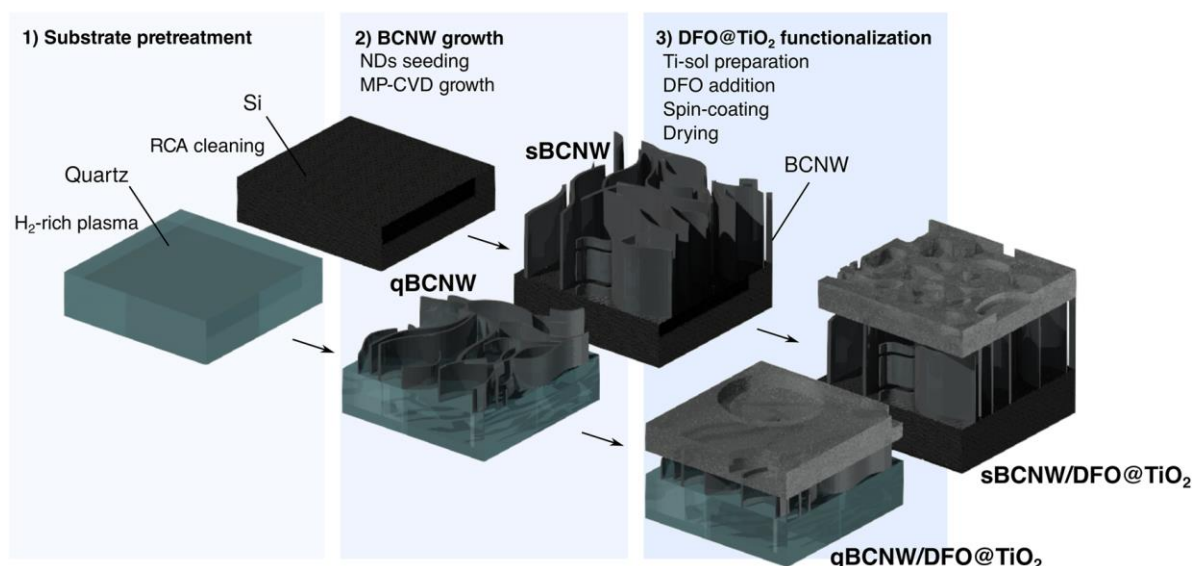


Figure 15. Electrochemically active materials [H7].

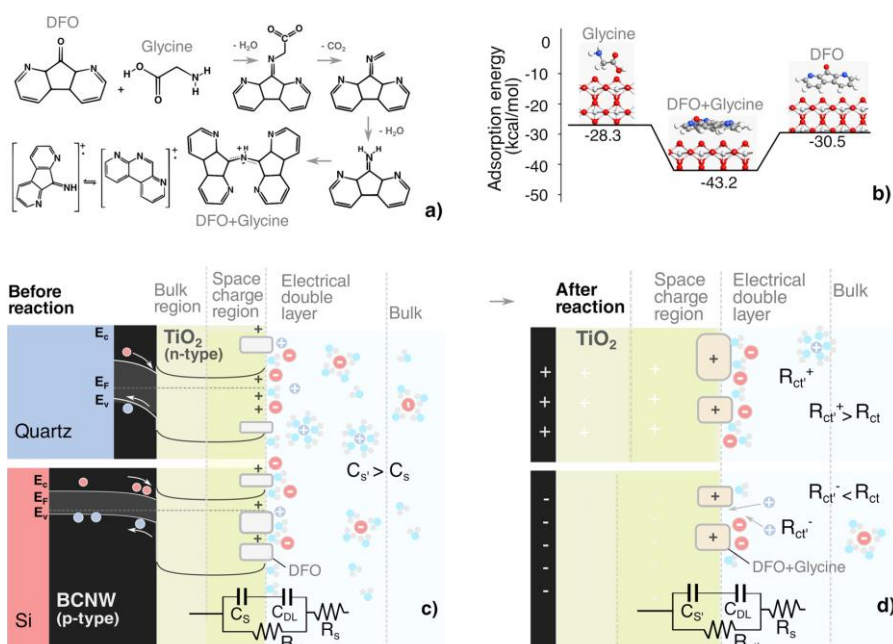


Figure 16. Electrochemical process flow on the obtained $\text{TiO}_2/\text{BCNWs}$ electrodes [H7].

The papers [H5, H7, T3] made important contributions to the development of structural analysis of polymer and carbon matrices and drugs/active compounds using Raman scattering spectra. Raman spectroscopy is a very well-studied method, the theory of oscillation-rotation spectra is the basis of many studies in quantitative and qualitative analysis, and the added advantage of the non-invasiveness of the method, and the lack of special sample preparation for measurements, makes it quite common in many laboratories. The Raman spectra presented as part of the publications [H9, H11] are an original contribution to the formulation of literature libraries of spectra for given materials with great application potential - Figures 17 and 18. They also play a key role in the development of modern forensic procedures for the rapid identification of drugs and prohibited substances in fingerprints [H11].

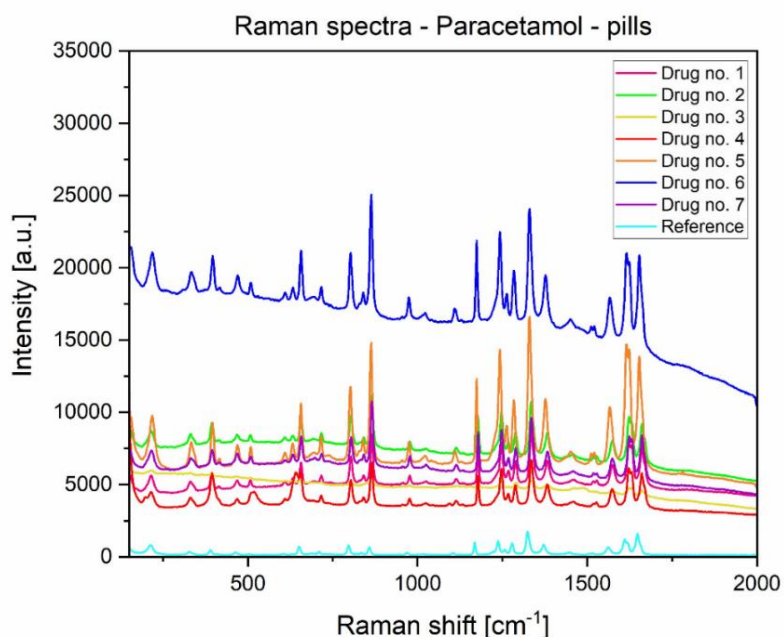


Figure 17. Raman scatter spectra for paracetamol as a reference substance and drugs from different manufacturers [H11].

I took advantage of the possibility of monitoring the polymerization of PVA films by selecting appropriate molecule structures and observing Raman scattering - Figures 18 and 19. The results are described in [H9], where, by synthesizing optically active PVA films, I "in situ" incorporated two different drugs (with different structures, and different spectroscopic properties) which influenced the arrangement of hydroxyl groups in the PVA matrices, and then significantly affected the diffusion processes of the molecules into aqueous solutions [H9].

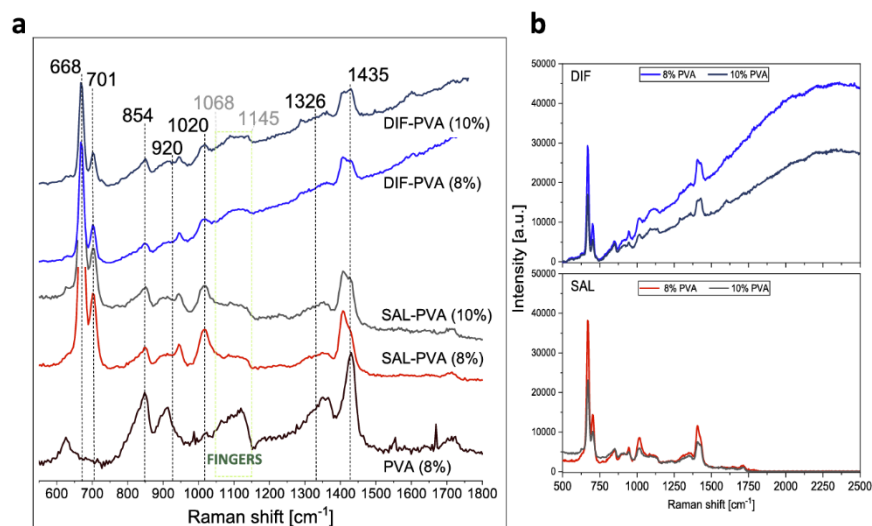


Figure 18. Raman scattering spectra for drugs in PVA polymeric materials [H9].

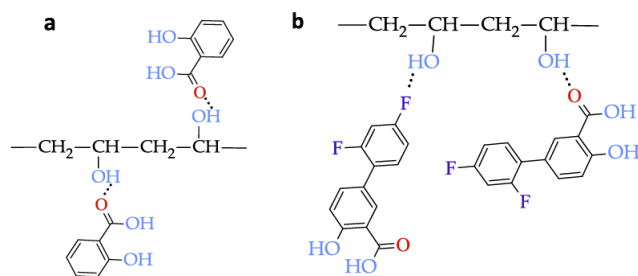


Figure 19. Structure of analyzed molecules in polymer matrices [H9].

Part of my work on the molecular workshop is the elaboration of physicochemical interactions in proteins responsible for Parkinson's disease, where I contributed to the interpretation of the physicochemical model and the analysis of the energy of the interactions between the active center of the enzyme-containing amino acids and the proposed drug inhibitor [H10]. **Identification of molecular mechanisms of interaction of PREP inhibitors affecting α -synuclein aggregation, which are responsible for the occurrence of neurodegenerative diseases, e.g., Parkinson's disease.** Knowledge of functional groups and the potential for interactions between active molecules relative to each other is important in molecular design.

The work [H10] is a continuation of research on optically active materials with applications also in medicine and pharmacology in connection with the issue of aggregation (formation of protein aggregates), which is one of the main causes of neuronal disorders and subsequent brain damage in many neurodegenerative diseases.

In Parkinson's disease, α -synucleins are responsible for the accumulation of aggregates. The origin of aggregation is unknown, but there is convincing evidence that it can be reduced by inhibition of proline oligopeptidase (PREP). Identifying differences in the dynamics of the enzyme inhibited by different compounds may lead to the identification of protein regions involved in the interaction between PREP and α synucleins - figure 20. In this study, we analyzed the effects of three PREP inhibitors, each of which affects α -synuclein aggregation to different degrees. Molecular dynamics modeling was used to identify the mechanisms underlying PREP inhibition and structural differences between the inhibitor-PREP systems were identified. Even subtle differences in the dynamics of the enzyme affect its interactions with α -synucleins, so identifying these regions may be biologically important in preventing α -synuclein aggregate formation - figure 21 [H10].

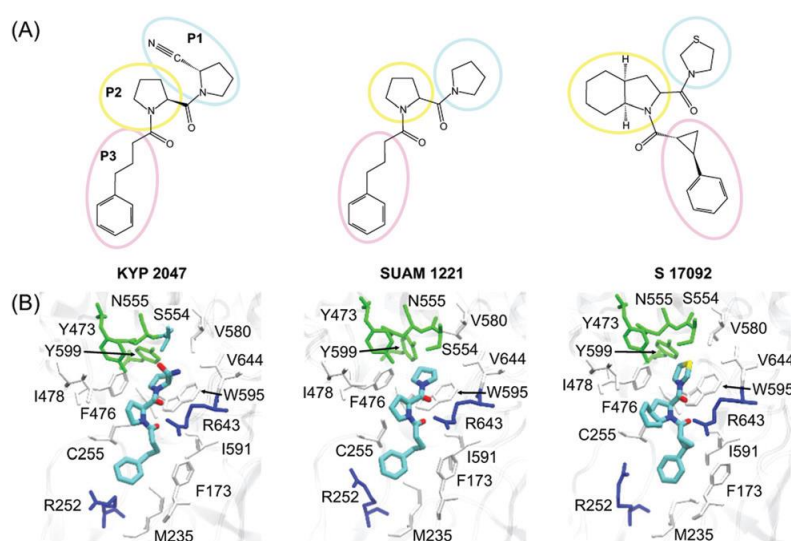


Figure 20. PREP inhibitors KYP 2047, SUAM 1221 and S 17 092, with the three reactive groups, P1, P2 and P3, highlighted (A), and structural fragments of the inhibitors and their surroundings for each system (B) [H10].

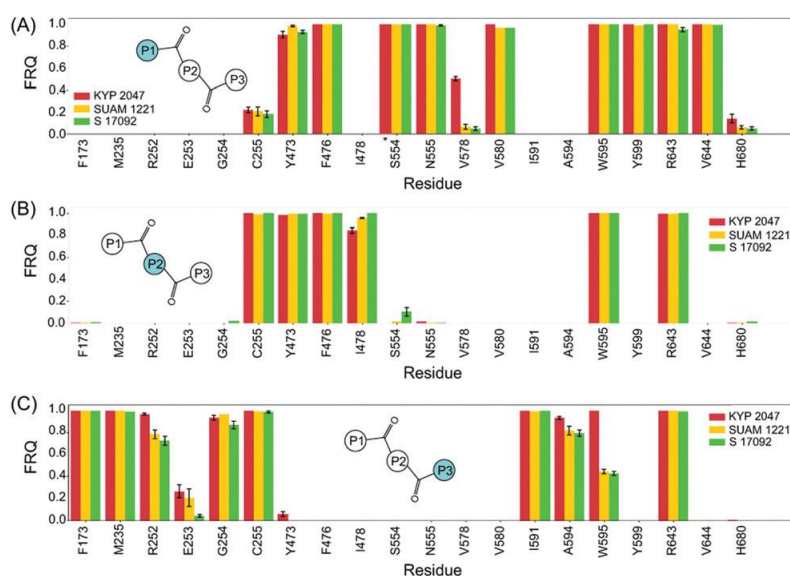


Figure 21. Schematic of the frequency of contacts between ligand functional groups and residues involved in their interactions [H10].

The acquired theoretical experience and observation of the complex structure of the enzymes responsible for Parkinson's disease has made a huge contribution to my further research path, where my current research is primarily based on the development of centers for fluorescent DNA or alpha-amino acid markers. My ongoing research is the design of hydrogel polymer films. Polymeric matrices are synthesized by a polymerization reaction, controlled by the type of polymer and external factors such as elevated reaction temperature and the addition of a catalyst or crosslinking agent, e.g., titanium dioxide, hydrogen peroxide, acetic acid. Figure 22 shows the research I am currently coordinating, i.e., methods to synthesize optically active materials using polymer matrices such as PVA, PVP, chitosan, and agarose with the addition of a luminescent probe. The main purpose of producing these materials is to visualize dactyloscopic traces and/or trace amounts of DNA. Analysis of the structure and photophysical properties of the materials obtained is made possible by using molecular physics techniques: UV/VIS spectrophotometry, steady-state and time-resolved spectrofluorimetry, fluorescence microscopy, and Raman spectroscopy. The results of research already received and currently in progress are an important contribution to the development of the presented discipline in the field of spectroscopic analysis and introduce innovative materials and procedures for molecular physics specialists.

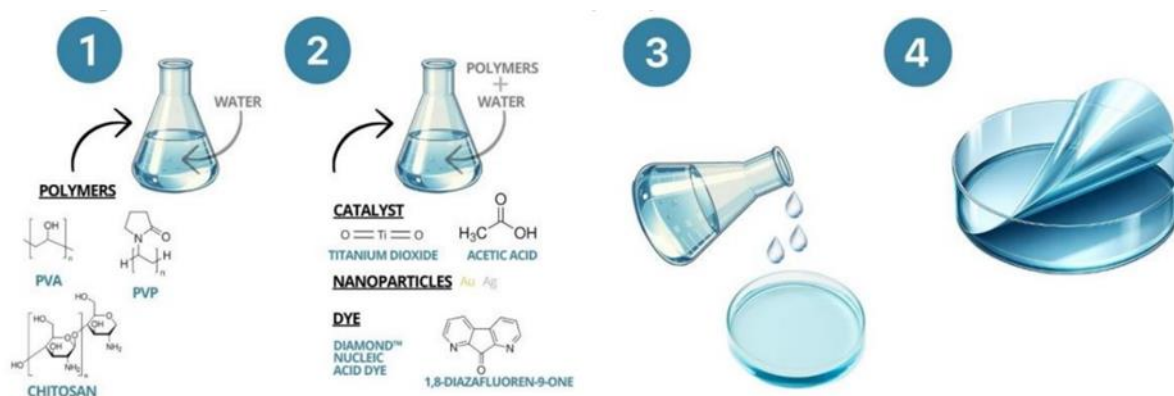


Figure 22. Methods for synthesizing optically active materials using polymer matrices such as PVA, PVP, chitosan and agarose with the addition of a luminescent probe [source: own development].

4. Molecular sensitization of a luminescent probe for α -amino acid identification using electron excitation energy

In the publication [H2], it was found that there are interactions between DFO molecules and solvent molecules of different polarity. Based on solvatochromic sensitivity studies of the DFO molecule, this electron transition was characterized. The physical data obtained enabled further work on the design of an optimal medium for the DFO fluorescence probe. The calculations performed indicated a clear **increase in the dipole moment in the excited state** especially for polar media, which was also confirmed by an increase in the intensity of the absorption band and a significant shift of these bands towards the infrared. This conclusion was very important during the molecular design of the subsequent centers for the DFO molecule. The research interest was directed toward **sensitizing the DFO molecule to the properties of the medium** in which it is located.

Sensibilization through appropriate matrix selection was also related to the chemical properties of DFO, which belongs to the group of **aromatic ketones**. Aromatic ketones exhibit specific synthetic properties, namely they are characterized by their ability to **cyclodimerize** [43-47]. This cyclodimerization, which was described in the publication [H12] in a completely innovative way, uses a previously unknown spectroscopic approach for the synthesis of sensitized materials. However, I emphasize that my experimental idea stemmed from previously confirmed literature reports on the formation of excited state complexes (excimers and exciplexes) using energy transfer processes during electron excitation, ultimately obtaining the possibility of various photochemical reactions. In this part of the thesis, I have mainly described **a novel approach to the possibility of sensitization of a molecule both spectroscopically/luminescently and electrochemically, while taking into account the diversity of energy loss processes after the electron excitation event** [48-50].

In the work [H3], I observed significant changes in the fluorescence spectra profiles with increasing concentration. I confirmed the influence of the matrix on the observed fluorescence of the DFO molecule. The emission of the monomer and the weakly fluorescent TiO₂ matrix (revealed by time-resolved measurements), was in a similar spectral region, although with low intensity for TiO₂ [51]. The increase in the fluorescence signal intensity of the monomer at low DFO concentration indicated the influence of the TiO₂ matrix. However, a decrease in the intensity of the monomer fluorescence signal at high DFO concentrations indicated the formation of fluorescent aggregates, DFO being solvatochromic sensitive and therefore a spectral shift effect could be expected with some changes in matrix polarity. However, the matrix remains chemically unmodified for all samples, and the effect of significantly changing the polarity of the entire matrix just by increasing the concentration of DFO molecules is improbable. The localization of the fluorescence band of TiO₂ compared to the fluorescence of DFO and other fluorene-like molecules in liquid solutions [H2,52,53] suggests that the TiO₂ matrix belongs to relatively non-polar media. This is also in line with other results and discussions conducted previously [54,55,56].

To gain more insight into the photophysical properties of the fluorescent forms of DFO, average fluorescence lifetimes were determined from fluorescence decay measurements for different concentrations of DFO - Table 3 in the paper [H4]. It was observed that fluorescence lifetimes shortened with increasing dye concentration, indicating the significant presence of aggregates, which may play a dual role in the system: first, aggregates may act as perfect or imperfect traps for excitation energy transferred from monomers [57-63], and second, aggregates at the highest concentrations may contribute to the fluorescence signal by emitting short-lived fluorescence. Similar behavior has been previously observed and analyzed for several other dyes such as rhodamine and carbocyanine in polymers and hybrid matrices, except that in this work the shift in the fluorescence spectrum was more pronounced [64,5].

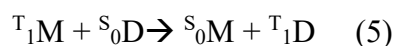
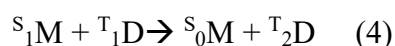
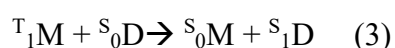
I drew an important conclusion, namely that the increase in the degree of aggregation was induced by hydrogen bonds (O-H...N). This was probably due to the formation of intermolecular hydrogen bonds between DFO and ethanol, water, or isopropanol molecules (the solvent remained in the TiO₂ pores after the sol-gel process). As a result, the molecules were able to combine with neighboring molecules and form aggregates. Meanwhile, the degree of aggregation increased as the concentration of DFO molecules in the thin films increased. These spectral changes were only observed in TiO₂ thin films and could be attributed to aggregate formation promoted by the TiO₂ matrix.

I observed enhanced solid-state luminescence with TiO₂ thin films in the presence of aggregates at high DFO concentrations. The aggregation process of DFO in the TiO₂ matrix, at sufficiently high concentrations, develops rapidly. I have confirmed using various complementary spectroscopic and microscopic techniques that the aggregates formed can emit short-lived fluorescence. The aggregation process is promoted both by the local surroundings of the DFO molecules to the TiO₂ nanochannels and pores, and by the presence of residual solvents that affect the ability of DFO to aggregate into larger structures. At high DFO concentrations, aggregates were formed, which affected the fluorescence emission. I observed an increase in fluorescence intensity with increasing DFO concentration in TiO₂ thin films (short-lived fluorescence). I indicated that the specific average lifetime of DFO fluorescence at high concentrations is also related to the presence of non-fluorescent DFO aggregates. In this work, I postulated the mechanism of electron transfer of excitation energy in sensitized rigid systems.

Published work [H4, H5, H6, H8, H12] clearly indicates that different types of electron states may be involved in the energy transfer and that the energy transfer may be in the mode of different interaction mechanisms between the monomer and aggregate molecules. I have postulated that **in the case of DFOs, primarily singlet states play an important role in energy transfer**, while **in rigid matrices, the activation of triplet states should be considered**. A novel use of biocompatible polymers as stable matrices for DFOs, where, by controlling the concentration of the DFO molecule, materials with stable photophysical properties of the newly formed dimer, emissively active in the new band (on the long-wave emission side of the monomer), were obtained. Of course, according to the so far known principles of photophysics, I take into account the possibility of energy transfer from the monomer to the dimer (cyclodimer) or higher-order aggregates present in the rigid matrices studied, according to the following equations (2), (3), (4), (5) and the diagrams shown in Figure 23:

Where S - singlet, T - triplet, M - monomer, D - dimer, 0 - basic electron state, 1- first excited electron state, 2 - second excited electron state

$S_1M + S_0D \rightarrow S_0M + S_1D$ 2) this is the most likely postulated mechanism [57,58]



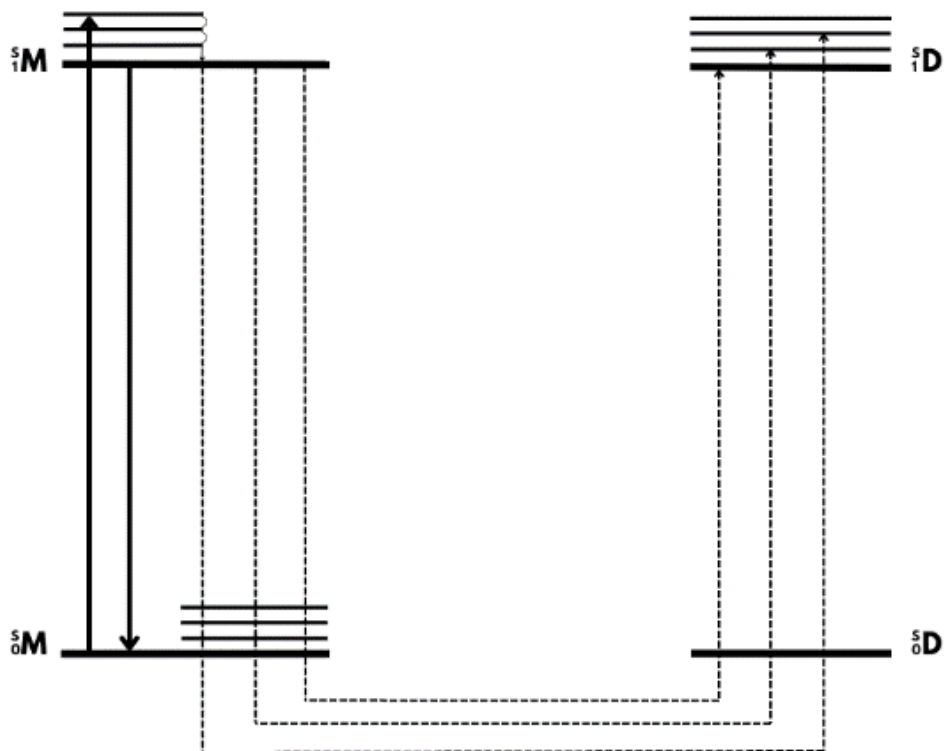


Figure 23. (2) Postulated excited state energy transfer mechanism [57,58].

The other mechanisms (2), (3) and (4) in rigid matrices, are also possible due to the probability of obtaining a triplet state.

The most efficient excitation energy transfer processes are those that occur when the spin of the monomer-dimer molecule system is conserved. The observed **singlet-singlet excitation energy transfer was confirmed by concentration quenching of photoluminescence**, and earlier work by other authors also confirms this type of mechanism as the leading one [65,66]. The presented schemes of the pathway of radiation-free energy transfer from monomer to aggregate (including dimer (cyclodimer)) are of great value from the point of view of applications in the process of revealing forensic traces (here primarily dactyloscopic traces and DNA traces). **I emphasize that triplet-singlet energy transfer also occurs in this type of system and is a competitive alternative to the use of fluorescence and phosphorescence phenomena.** It should also be emphasized at this point that, despite spin-excited transitions, energy transfer can occur because it follows the selection rules for exchange-resonant energy transfer. The optically active materials I have proposed with these spectroscopic properties represent a potential material for use in the forensic laboratory for revealing/visualizing forensic traces and securing documents or banknotes.



Figure 24. Schematic of possible energy transfer pathways in optically active materials/centres [source: own development].

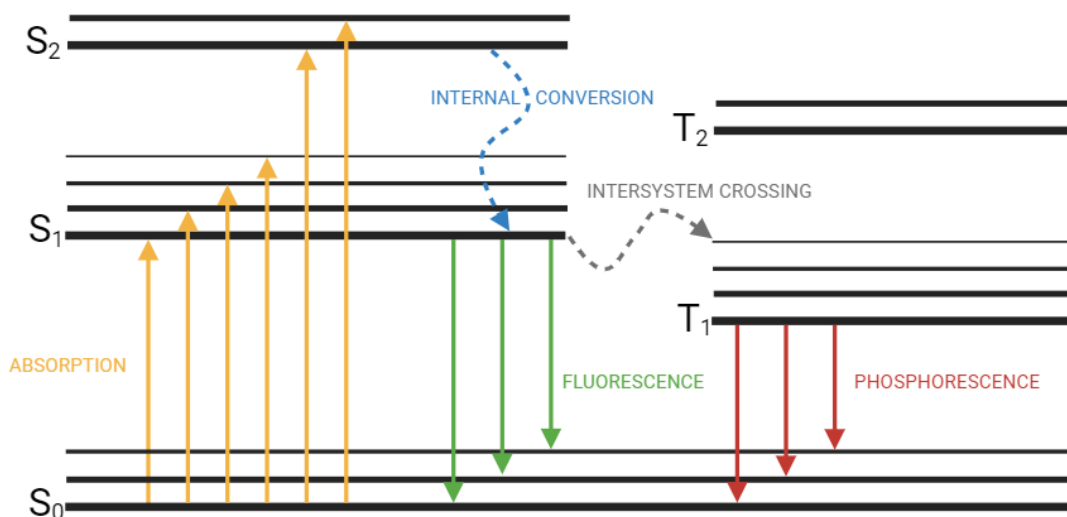


Figure 25. Diagram of the Jablonski Diagram with the presentation of the Deactivation of Excited States Energy [source: own development].

Sensitized fluorescence of the acceptor monomer DFO can be observed for rigid matrices with a dye concentration of about 10^{-3} [M], because for this concentration the number of molecules (DFO) in 1 cm^3 is equal to 6×10^{17} , so the average volume per molecule (DFO) is $1.4 \times 10^{-18} \text{ cm}^3$, i.e. for the volume of a sphere, we have a radius of 7 nm. In rigid matrices, there are no discrete oscillatory levels, and in the gaseous state and in solutions with low DFO concentrations, the process of establishing thermal equilibrium between the oscillatory energy of the donor and the environment (medium) is much larger than for rigid matrices, where the electron energy transfer process is much faster.

In [H12], I showed that there is a low probability of energy transfer by DFO (monomer) molecules in the triplet state, because the energy of the donor (DFO monomer) triplet state is smaller (2.28 eV) than the energy of the acceptor (2.39 eV) triplet state (DAK DFO dimer). The energy values were obtained from quantum mechanical calculations. In this case, the analysis of experimental absorption or emission spectra was not used alone, because, for structures as complex as DAK DFO, it is possible to change the equilibrium geometry of the molecule and the assumption that the origin of the spectrum is the (0,0) transition may be incorrect. Thus, in this case, the photosensitization efficiency is 0. However, returning to the possibility of changes in the equilibrium geometry of the molecule, the literature has identified a cis-stilbene molecule [67] where, although the energy of the donor is lower than that of the acceptor in triplet states, it is likely that changes in the equilibrium geometry of the acceptor occur during excitation. In the calculations, we also note the position of T_2 just below the S_1 level for the DFO monomer (donor) and the position of T_3 just below the S_1 level for the DAK DFO dimer (acceptor). Moreover, the process of internal conversion from the T_2 to T_1 state (monomer) and T_3 to T_2 and from T_2 to T_1 (dimer) is forbidden, due to the $u, \leftarrow/\rightarrow g$ selection rule, so the resonant energy transfer process may also be a very important energy transfer mechanism here, which can be controlled by optimizing the external environment of the molecule and its physicochemical tendencies towards different types of chemical processes and changes in photophysical properties. The mechanisms of the various photophysical processes after the photon absorption by the molecule has occurred are illustrated in Figure - 24 and Figure - 25. These figures fully capture the complex structure of the energy transfer mechanisms by the considered DFO molecule in different matrices.

4.5 Molecular aggregation - a physical aspect in molecular design

Organic aggregates currently play a significant role, mainly due to their unique, often specific photophysical and optoelectronic properties in the aggregated state. These properties are linked to the structure of the aggregates and the way they are molecularly packaged. In the literature, H and J aggregate models defined on the basis of the molecular exciton model have long been known. On the other hand, we have unconventional aggregates, which include induced aggregation emission (AIE) systems. In the paper [H8], I present the possibility of forming an AIE and its impact on the surface energy characteristics of the materials. All materials have been prepared as hybrid biocompatible thin films in which the matrix is TiO_2 or TiO_2 /carbon nanowires (CNWs) with an embedded dye in the form of 1,8-diazafluoren-9-one (DFO).

I have presented the propensity of DFO to aggregate and characterized the internal energy of the dye in several aggregated structures using quantum chemistry calculations. The results highlight that DFO is an attractive structure for the design of new fluorophores due to its low molecular weight, the presence of a nitrogen atom that provides good coordination

properties, and its ability to form hydrogen bonds. Our studies show that using suitable matrices, i.e., rigid supports, creates preferred aggregate forms in the excited state with high emission efficiency in the band maximum around 550 nm.

Many authors have described the process of aggregation of molecules in solution and analyzed the influence of various factors on aggregation processes [8,9,10,68-75]. These works have shown, among other things, that an important factor influencing the probability of aggregate formation is the concentration of the dye, and, from a practical point of view, it is possible to speak of a limiting concentration below which aggregation of dye molecules is barely visible and considered insignificant. In the case of rhodamine 6G in aqueous solutions, this concentration is as low as 10^{-5} [M], whereas for solutions in which the solvent is glycerol, a change in the absorption spectral profile is noticeable at concentrations higher than 10^{-2} [M] [76]. According to the results presented in the above work, the size and structure of the aggregates strongly depend on the environment in which the molecule resides and the concentration of the dye. Other factors that have a significant influence on the aggregation process in different systems are the amount of electrolytes, surfactants, additives, chelating agents, the chemical structure of the dye, and external factors such as temperature and pressure. Nowadays, due to the diverse applications of pure dye materials, quantitative and qualitative control of the aggregation process is important. Furthermore, it is worth pointing out that aggregation processes are often overlooked in the interpretation of spectroscopic properties, as evidenced by current procedures for visualizing dactyloscopic traces with DFO. DFO working solutions contain high concentrations of DFO, and not only DFO complexes with amino acids but also DFO aggregates are involved in the visualization of dactyloscopic traces, as indicated by our previous work [**H4**, **H6**, **H8**, **H12**].

In the present work [**H4** and **H8**], time-resolved spectroscopy shows new possibilities to reveal short-lived (fast) processes that are not visible in stationary spectroscopy. The time evolution of the spectrum allows us to observe significant changes in the spectroscopic properties of the dye. The results obtained with this ultra-sensitive method led us to another possibility, namely, to try to relate the changes in spectroscopic properties for short-lived processes with the change in energy at the surface of thin film matrices. In earlier work, I have pointed out the ability of DFO to aggregate [**H4**, **H5**, **H6**, **H8**]. At the same time, I shifted the interpretation towards the presence of unconventional aggregate structures that exhibit the ability to fluoresce. Moreover, they enhance the emission of the structures under consideration. The literature gives examples of other molecules responsible for the formation of unconventional aggregates with the ability to emit fluorescence [45,46,47,48].

However, the possibility of using enhanced emission to produce biomaterials, in which aggregation processes of biologically active molecules can be controlled and used to reveal, among other things, α -amino acids, which are important markers for many biochemical processes occurring in living organisms, has not been previously described. I have presented an energy diagram of such aggregates - aggregation-induced emission (AIE) - in Figure 26.

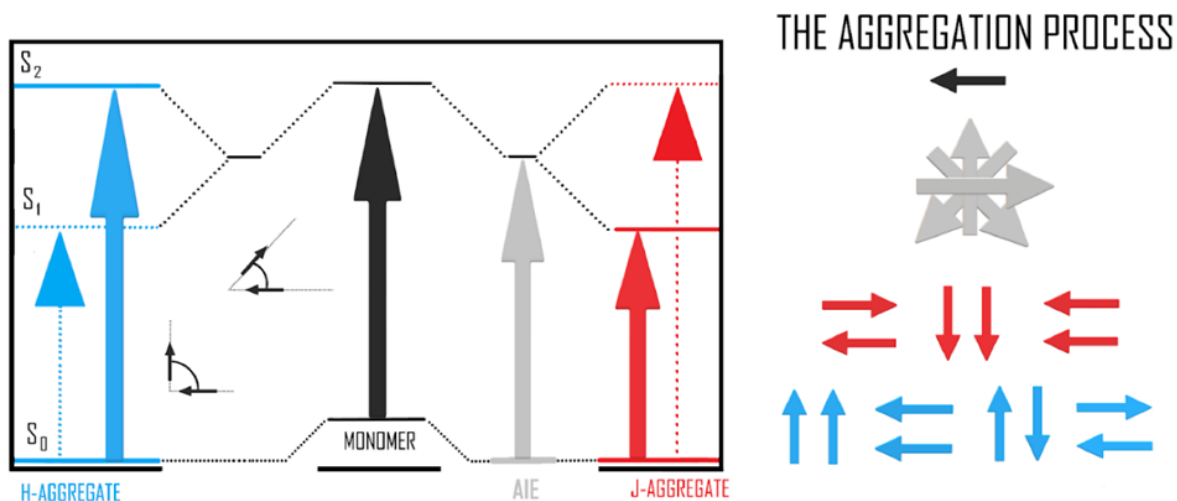


Figure 26: Energy diagram of the aggregates [H8].

AIE aggregates are structures that are π -conjugated organic molecules and show weak or negligible fluorescence in dilute solution, but in solid, rigid matrices we observe enhanced fluorescence from these structures [77-79]. DFO is one of the molecules characterized by π -conjugated organic molecules. It is worth mentioning that a variety of intermolecular interactions (i.e. $C\cdots O$, $O\cdots O$, $C-H\cdots O$, $C-H\cdots C$) are the main interactions that provide a natural drive to consolidate the corresponding conformations of molecular aggregates and lead to the chromophore in the solid state being highly emissive. In the case of DFO in TiO_2 and TiO_2/CNW matrices, we observe the formation of highly emissive dyes (450 nm to 550 nm). In turn, computer calculations allowed me to identify the most stable aggregate conformations and directly relate these results to the interpretation of the parameters characterizing the surface energies of DFO thin films in two types of matrices: TiO_2 and TiO_2/CNW s. Furthermore, using quantum mechanical calculations, I confirmed the energetic tendency of the DFO molecule to aggregate with a preference to form a dimer structure. This result is in strong agreement with the results of our recent publications [H6], in which we confirmed the aggregation ability of DFO in ethanol and the emission of DFO aggregates in ethanol with an emission maximum at a similar wavelength as the DFO complex with glycine (an α -amino acid). These results significantly affect the application of DFO in fingerprint analysis and allow us to predict the use of DFO on different types of substrates with different surface energy characteristics.

I would also like to highlight here a particularly important physical aspect in the form of molecular spectra directly related to the presentation of the molecule aggregation phenomenon. My recent experimental and theoretical research in the interpretation of molecular spectra clearly shows great progress in this field, moreover, their effect serves to present the molecular structure and there is no competing method to indicate the detailed physical characteristics. A more detailed spectroscopic knowledge allows an understanding of the molecular structure and thus makes it possible to apply it to different regions in the form of luminescent probes or excitation energy carriers. Some of the important molecular processes of interest in the publications are association/aggregation processes and the possibility of 'in situ' reactions when optimizing the concentration of a dye in the matrix being analyzed.

Within the scope of this work, I present the influence of these processes on the mechanisms of concentration quenching of photoluminescence, which can be determined by the presence of spectroscopically active dimers (rigid materials). We assume that there are two types of spectroscopically active molecules in films: the DFO monomer and the DAK DFO dimer [H12].

Whereby the law of action of masses holds:

$$C'' = K \cdot C'^2; (6)$$

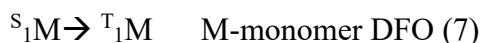
K - dimerization constant

C' - monomer concentration

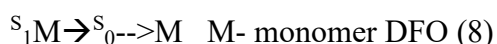
C'' - concentration of the dimer

Postulating the fluorescence activity of dimers, concentration quenching of photoluminescence is therefore primarily due to the non-radiative transfer of excitation energy from monomers to dimers. By treating the dimers as an energy acceptor and using a donor concentration (monomer DFO) much higher than the acceptor concentration, we are dealing with conditions that favor non-radiative excitation energy transfer, which is manifested by concentration quenching of photoluminescence [80-85]. However, monomer fluorescence in solutions has been observed, but dimers are not fluorescently active, while fluorescence activity of DFO aggregates has been observed in thin films and polymer films.

Previous studies by other authors have clearly shown that the dimerization process is influenced by the water content [65] in our systems, ethanol, and the type of matrix, i.e., increasing its rigidity, played the greatest role. In addition, application studies also showed the influence of another compound. The overriding factor, however, was the type of molecule analyzed, which showed under conditions specifically optimized for it the ability to cyclodimerize. However, it should be emphasized that the quenching process is also the result of transitions, where the electron excitation energy is converted irreversibly into vibrational energy [86]. Moreover, the analyzed DFO monomer molecule, in every environment considered, shows a low, almost zero absolute fluorescence quantum yield at room temperature, confirming that the electron excitation energy is transformed into thermal energy. The mechanism of excitation energy transfer considered for the DFO molecule in various matrices from gases to solutions and viscous rigid systems in the form of thin films and polymer films is very complex.



Or less likely by internal conversion



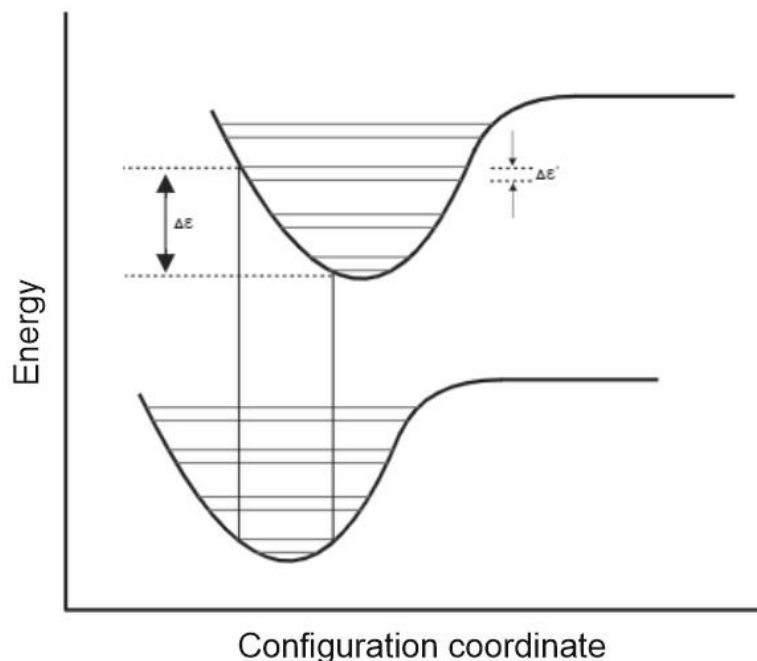


Figure 26. Potential energy curve [source: own elaboration].

The cases considered in the publications [H4, H5, H6, H8, H12] note that the efficiency of electron degradation of the excitation energy depends on the wavelength of the excitation light, the type of medium, the chemical-structural properties of the molecule, the possibility of aggregation complexation or cyclodimerization reactions occurring. The above work also supports the concept of earlier [87-88] that the probability of non-radiative transitions depends on the Franck-Condon factor of the density of the final states, but under the condition of the same energy as the initial state - Figure 26.

The aggregation process is clearly reflected in the tracking of **luminescence quenching processes**. Photophysical analysis of the quenching process plays an important role during the molecular design of optically active materials. This process is observed by interpreting fluorescence lifetimes in the excited state, namely by its shortening. The mechanisms for the occurrence of this process are usually complex but can be controlled and optimized to the needs of the photosensitization process. In the case of the articles presented here, the important effects of the formation of fluorescent aggregates and stable complexes of DFO molecules with α -amino acids [H4, H5, H6, H8] or the cyclodimerization process on luminescence quenching [H12] were described. The intermolecular processes considered within the scope of this work involving the excited DFO monomer molecule primarily involve electron transfer and association with the formation of permanent bonds in the form of the DAK DFO cyclodimer and short-lived bonds in the form of hydrogen bonds between DFO and solvents of high polarity (with hydroxyl groups). Especially notable are **rigid matrices** as a medium for DFO molecules, where the luminescence is not observed to be completely extinguished, as it is complemented

by the luminescence of newly formed active molecules in the system - Figure 27. The aggregation phenomenon is a physical process that, when properly controlled through the use of methods and procedures from the field of molecular spectroscopy, allows the design of matrices with the required application properties.

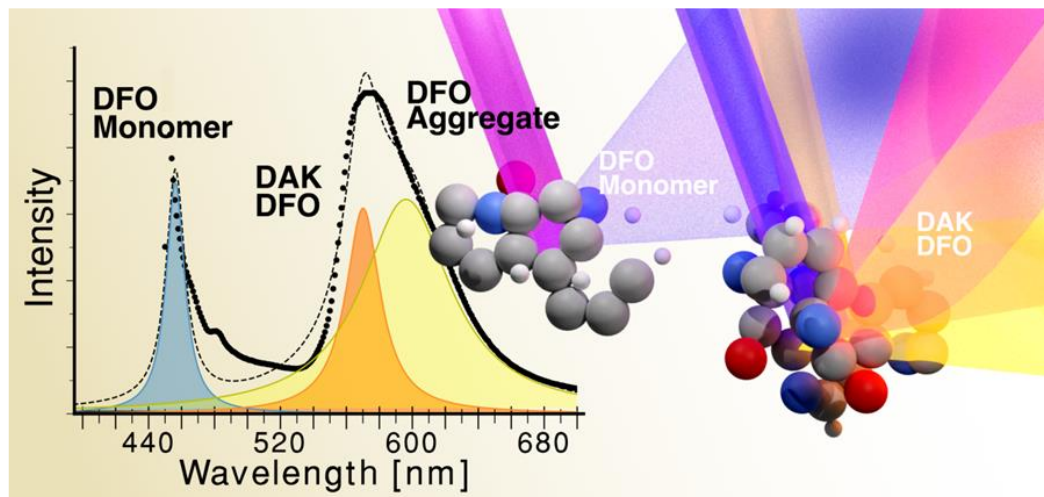


Figure 27. Fluorescence spectra of DFO monomer, DAK DFO cyclodimer and higher-order DFO aggregates [H12].

4.6 Summary

This present work includes the results of experimental and computational studies that deal with the effect of concentration on some photoluminescence properties of solutions and rigid systems. Within the context of papers H1-H12 and P1, my contribution was a presentation on the topic:

- **Interpretation of the physical processes of concentration and extinction of fluorescence (photoluminescence) occurring in the systems under consideration, characterized by different structural-spectroscopic features.**
- **Solvatochromic effect for the molecule 1,8-diazafluoren-9-one (DFO) in solutions and rigid matrices such as titanium dioxide and biocompatible polymers PVA, PVP.**
- **Demonstration of the changes in photophysical and chemical properties to which the DFO molecule is subjected depending on the local environment.**

The lowest excited singlet state of the molecule (n, π^*) was observed in the explored DFO molecule in low-polarity media. In contrast, the lowest-energy state (π, π^*) was found to be located at a higher energy level in the same molecule when dissolved in a solvent of high polarity. This arrangement of levels was found to be reversed when DFO was dissolved in a solvent of high polarity, especially in the presence of the possibility of forming hydrogen bonds. Considering the distance of levels (π, π^*) between the state S and T, we obtain much higher energy values for the states (n, π^*) between S and T. The distance between states T (n, π^*) and (π, π^*) is smaller in a sequential manner, as evidenced by our quantum mechanical calculations [H12]. Consequently, these levels are highly sensitive to any changes in the external environment. Previous studies of cycloaddition reactions between cyclopentanone and alkenes,

which yielded cyclobutane derivatives, proposed the involvement of T2 triplet states in the reaction [89]. The presented spectroscopic studies on the DFO molecule demonstrated that electron excitation in this case (of an aromatic ketone) can result in a multitude of complex chemical outcomes.

Controlling the environment of the molecule is the key to controlling the parallel states between competing photophysical and chemical processes. Rigid matrices, which have received the most attention in published works [H4, H5, H6, H8, H12], exhibit completely different physical and chemical mechanisms after excitation of the molecule than in the gas phase. In the gas phase, the oscillatory energy after excitation is critical for the occurrence of a given chemical process.

In rigid systems, we have competitive processes in the form of energy transfer processes or two-molecule cyclodimerization of an excited DFO molecule. The type of the lowest excited electron state and the type of occurrence of the eventual chemical transformation in the case of DFO changes with the change in the polarity of the medium [H6]. Ethanol and water were chosen as the leading solvents in rigid systems for further application studies. This base bond was used for further molecular design activities, where the type of polymer or precursor was changed in the system, but the environment of the molecule was controlled in the primary mode through the medium of ethanol and/or water.

- Develop a comprehensive procedure for the analysis of the DFO molecule in terms of molecular physics, from the synthesis of materials to the preparation of structural and photophysical characterization.

- Demonstrated the possibility of a pathway for radiation-free energy transfer from excited monomers to non-illuminating dimers - a phenomenon observed for DFO in solution, but also for TiO₂ matrices.

- The presentation of variants of the application of molecular characterisation of aggregation phenomena in solutions and rigid systems to real systems on the basis of molecular physics has led to the application of these results already in the real model in the form of a physical method for revealing/visualising dactyloscopic traces on plain and thermal paper - National Patent Application.

In presenting and interpreting my research, I also highlight unique collaborations with theorists. Molecular simulations and modelling have an invaluable impact on the interpretation of molecular interactions in newly synthesised matrices for spectroscopically active molecules. In the work presented here, I have focused primarily on condensed matter, so-called rigid materials. Molecular simulations have provided an understanding of the spectroscopic properties that are key to further application efforts. The emergence of disciplines such as chemical, biomolecular, cellular and tissue engineering has led to the necessity for molecular physics to consider the possibility of advanced syntheses or the processing of materials when optimising the environment for a luminescent probe during photophysical analyses. The work addresses topics related to sustainability, manifesting itself in the optimal use of applied spectroscopic procedures to obtain new compounds in so-called 'clean chemistry'. Moreover, the application of procedures that minimise the toxicity of the compounds used contributes significantly to addressing topics related to respect for the environment and reducing the number of chemical compounds used, which are part of the global challenge currently facing humanity.

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5. Presentation of significant scientific or artistic activity conducted at more than one university, scientific or cultural institution, especially at foreign institutions

5.1 Accomplished scientific and research achievements, including cooperation with other scientific institutions.

- a) Establishment of the Forensic Trace Detection Laboratory at the Faculty of Law and Administration of the University of Gdansk as part of the development of Forensic Science in Pomerania and the Patent Application obtained in the Forensic Trace Detection Laboratory.

The high level of teaching activity in the field of applications of physical methods in forensic science provides a strong motivation for me to engage in research activities, particularly in the context of the application of scientific activities and their practical applications in this field. At present, I am a co-author on a significant research project that is innovative and unique due to its interdisciplinarity and the form of cooperation between representatives of the physical sciences and legal sciences. The project, entitled "New Physicochemical Methods of Revealing Dactyloscopic Traces as a Forensic Tool for Increasing the Efficiency of Crime Detection in the Criminal Process (2021/41/B/HS5/03250)," represents a pioneering forensic tool. This project is carried out in collaboration with the Faculty of Law and Administration of the University of Gdansk, under the leadership of Professor Krzysztof Woźniewski. It comprises two parts: a legal and a physical-chemical one. It was a key stage in the establishment of the Forensic Trace Detection Laboratory. In the physical-chemical part, I am a coordinator of laboratory activities aimed at developing an innovative procedure for the visualizing of fingerprint traces. As a result of this collaboration, the first patent application, for which I am the author, was created: "Method of visualizing dactyloscopic traces and solution for visualizing dactyloscopic traces." The joint research aims to develop laboratory and legal procedures for human identification, an important aspect in the field of forensic sciences, and makes innovative use of molecular physics.

The original scientific and research achievement, which was realized through the establishment of the Forensic Trace Detection Laboratory, received significant support from the Dean of the Faculty of Law and Administration of the University of Gdansk and the Dean of the Faculty of Mathematics, Physics and Informatics of the University of Gdansk. However, it is important to note that this project represents a scientific initiative in which I act as the coordinator and main author. The achievement consisted of the comprehensive equipping of the laboratory with physicochemical equipment, including both basic apparatus and advanced equipment for research in the field of molecular spectroscopy.

The laboratory has been equipped with specialized apparatus for the synthesis of thin films and foils, utilizing techniques such as sol-gel, spin-coating, and the broad polymerization process. Additionally, the laboratory has been equipped with equipment for DNA analysis, including apparatus for carrying out the electrophoresis process and polymerase chain reaction, as well as professional forensic illuminators.

It is noteworthy that these investments represent a distinctive contribution to the advancement of fluorescence applications in forensic science. The laboratory has contributed to the development of molecular analysis, with a particular focus on molecular design using molecular physics. The research conducted within the Forensic Trace Detection Laboratory is motivated by the rapid advances in design and develops innovative

approaches that indicate the possibility of controlling excited state deactivation processes by weakening absorption from the S0 to S1 state and enhancing direct absorption from the S0 to T1 state- a collaboration with Prof. Ignacy Gryczynski and Prof. Zygmunt Gryczynski of Texas Christian University. It is commonly assumed that the probability of transitions from the S0 state to T1 is negligibly small due to the intercombination prohibition and the large energy difference between these states. However, it has been demonstrated that strong mixing of states with different multipletities can, for selected fluorophores in certain solid matrices, significantly weaken the intercombination prohibition even for such states. As a result, directly excited long-lived phosphorescence-like emission can be observed at room temperature. This newly discovered physical effect is not only the subject of basic research, but also has significant potential for application in the field of forensics, including the revelation of forensic traces, such as fingerprint and DNA traces. In these studies, the background is an important input during typical visualization by the short-lived fluorescence method. The current method should allow a significant reduction in the level of this background, thereby facilitating more sensitive DNA detection.

Furthermore, I have initiated a collaborative effort with a team led by Professor Zygmunt Gryczynski in the utilization of molecular spectroscopy techniques. Our joint objective is the advancement of novel methodologies for the identification of individuals, with a particular focus on circumstances pertaining to victims of mass disasters within the context of international procedures. Professor Gryczynski is an expert in the application of fluorescence spectroscopy to the analysis of biological systems. He has collaborated and published with two Nobel Prize laureates: S. Prusiner (1997) and B. Kobilka (2013). It is important to highlight that my current research endeavors are highly interdisciplinary in nature, facilitating a synergistic integration of knowledge and practical skills derived from the domains of physical sciences, forensic sciences, and legal sciences. This approach plays a pivotal role in the attainment of research objectives.

My work and research achievements are also reflected in my collaboration with the research group of Prof. Robert Bogdanowicz of the Gdansk University of Technology. **My contributions to the field of molecular physics are utilized in optoelectronics research.** The research collaboration primarily involves publications in the fields of electrochemical sensors, active carbon platforms, and their spectroscopic characterization, with a focus on oscillation-rotation spectra [T2-T4]. The interpretation of Raman scattering measurement results is a challenge in the case of structures such as doped diamond films. The author of the habilitation has extensive experimental experience in the field of molecular spectroscopy, including the analysis of Raman spectra, which has resulted in numerous publications in this area. Moreover, the use of Raman spectroscopy for the analysis of fluorescence spectra with very low intensity and low fluorescence quantum yields has led to the proposal of a new test procedure for the identification of fluorescence spectra for emissive N-doped carbon structures. This method has been demonstrated to be competitive with time-resolved measurements of fluorescence spectra. The research also proposed state-of-the-art diagnostic electrode materials [T2-T4]. Electrochemical analysis has enabled the determination of the factors influencing the electrical properties of environmentally friendly electrodes and their application in the identification of alpha-amino acids and specific groups of drugs or banned substances. The measurement of the electrical signal serves as the foundation for proposed sensory platforms for the detection of alpha-amino acids and paracetamol [H7, T3]. The structural-spectroscopic characterization of materials in the form of boron-doped diamond (BDD) thin films has the potential to be utilized in the development of electrical and electrochemical sensors [T4].

b) Research conducted in collaboration with international partners and other scientific and research institutions in Poland.

As part of an international collaboration, I undertook a foreign internship at **C.N.R. Istituto di Biochimica delle Proteine, Naples, Italy** from 23 October 2012 to 18 April 2013. The result of the research internship was a joint publication: *A surface plasmon resonance based biochip for the detection of patulin toxin*, Optical Materials, Pennacchio, A.; Giuseppe Ruggiero, G.; Staiano, M.; Piccialli, G.; Oliviero, G.; **Lewkowicz, A.**; Synak, A.; Bojarski, P.; D'Auria, S. Volume 36, 10, August 2014, 1670-1675, doi.org/10.1016/j.optmat.2013.12.045. In this study, I participated in the research and design of a test procedure to characterise the conjugation of a novel patulin derivative with bovine serum albumin to produce polyclonal antibodies. Additionally, a novel competitive immunoassay for the detection of patulin was presented. This paper presents a detection methodology utilising an optical technique known as **surface plasmon resonance (SPR)**.

In addition, I was engaged in research at other research centres, including the Institute of Catalysis and Surface Physicochemistry of the Polish Academy of Sciences in Krakow and the Institute of Forensic Expertise in Krakow.

Between 21.06-26.06.2010, within the framework of research cooperation with a group of scientists from the **Institute of Catalysis and Surface Physicochemistry of the Polish Academy of Sciences** in Krakow, I co-authored three posters and one oral presentation at the 13th international conference on theoretical aspects of catalysis in Matsushima Ichinobo, Japan. The research was based on calculations in the VASP programme of photocatalytically active heteropolyacid structures.

My research experience was extended by joint research performed at the **Institute of Forensic Expertise** in Cracow in cooperation with Prof. Dr. Brożek-Mucha in the periods 11.2008-06.2009 and 07/08 2009- my tasks included taking measurements on the Scanning Electron Microscope with X-ray microanalysis, participation in an experiment for the disclosure and characterisation of post-shot particles - analysis in the time since the firing of Glock firearms and lead ammunition and collection of samples - environmental research, the phenomenon of metallic contamination with post-shot particles from persons who have professional or hobbyist contact with firearms.

c) I have participated in numerous research projects in which I have led or coordinated research in the field of molecular spectroscopy.:

I. External research projects:

1. Title: **In situ synthesis of a luminescent probe matrix of 1,8-diazafluoren-9-one in the form of a titanium dioxide thin film.**

Registration number: 2017/01/X/ST5/01541

Source(s) of funding: **NCN**

Grant's name: **MINIATURA**

Costs: 49 500 PLN

Implementing entity: University of Gdańsk; Faculty of Mathematics, Physics and Informatics

Starting date: 23.12.2017 Closing date: 22.12.2018

List of major publications resulting from the project:

Publications in journals:

Lewkowicz, A.; Bogdanowicz, R.; Bojarski, P.; Pierpaoli, M.; Gryczyński, I.; Synak, A.; Mońka, M.; Karczewski, J.; Struck-Lewicka, W.; Wawrzyniak, R.; Markuszewski, M. J. The Luminescence of 1,8-Diazafluoren-9-One/Titanium Dioxide Composite Thin Films for Optical Application. *Materials* 2020, 13 (13), 3014. <https://doi.org/10.3390/ma13133014>. **140 points, IF (3.057)**

Texts in post-conference publications:

Lewkowicz, A.; Synak, A.; Mońka, M.; Bojarski, P.; Szczodrowski, K.; Bogdanowicz, R.; Karczewski, J. SURFACE and SPECTROSCOPIC PROPERTIES of 1,8-DIAZAFLUOREN-9-ONE in TITANIUM DIOXIDE THIN FILMS. *International Symposium on Molecular Spectroscopy 2018* 2018. <https://doi.org/10.15278/isms.2018.th09>.

2. Title: **New physico-chemical methods of revealing dactyloscopic traces as a forensic tool for increasing the efficiency of crime detection in criminal proceedings**

Registration number: 2021/41/B/HS5/03250

Source(s) of funding: NCN

Grant's name: OPUS-21

Costs: 898 408 PLN

Implementing entity: University of Gdańsk, Faculty of Law and Administration
During implementation - contractor and coordinator of the experimental part

Starting date: 18.01.2022 Closing date: 17.01.2025

List of major publications resulting from the project:

Publication 1:

Lewkowicz, A.; Kantor, M.; Zalewski, W.; Bojarski, P.; Mońka, M. Spectroscopic Evidence of Fluorescence by 1,8-Diazafluoren-9-One Aggregates—a Prospective New Ultrasensitive Method for Fingerprint Trace Detection. *Journal of Forensic Sciences* 2022, 67 (4), 1468–1475. <https://doi.org/10.1111/1556-4029.15039>. **70 points, IF (1,717)**

The publication includes the required acknowledgements to NCN.

Publication 2:

Lewkowicz, A.; Pierpaoli, M.; Walczewska-Szewc, K.; Czarnomska, M.; Bojarski, P.; Bogdanowicz, R.; Pogorzelski, S.; Kułak, L.; Karczewski, J. Nonconventional 1,8-Diazafluoren-9-One Aggregates for Green Light Enhancement in Hybrid Biocompatible Media. *Materials* 2022, 15 (14), 5012. <https://doi.org/10.3390/ma15145012>. **140 points, IF (3,748)**

Publication 3:

Pierpaoli, M.; **Lewkowicz, A.**; Dec, B.; Nadolska, M.; Bogdanowicz, R. Impedimetric Sensing of α -Amino Acids Driven by Micro-Patterned 1,8-Diazafluoren-9-One into Titania- Boron-Doped Maze-like Nanocarbons. *Sensors and Actuators B: Chemical* 2022, 371, 132459. <https://doi.org/10.1016/j.snb.2022.132459>. **140 points, IF (9,221)**

II. Internal research projects-project manager:

1. BW Investigation of the photophysical properties of 1,8-diazafluorenone (DFO) as a biosensor for genitourinary cancer markers

Project duration: 1.06.2017 - 31.12.

The aim of the project was to investigate the photophysical properties of 1,8-diazafluorenone as a biosensor complexed with potential markers of genitourinary cancers.

The current research in this area is based on complementary analytical measurements using gas chromatography (GC) and liquid chromatography (LC) methods, and the definition of a numerous group of substances whose levels in biological material change depending on the presence of cancer cells. Individual biomarkers have been proposed in the literature, e.g. for prostate cancer, but their effectiveness as diagnostic indicators are quite low. The project proposes to further select metabolites whose levels in urine samples may indicate the presence of genitourinary cancers, through an innovative spectroscopic-synthetic approach that will assess the enhancement or appearance of luminescence of potential metabolic markers. The application of steady-state and time-resolved spectroscopy techniques will permit the determination of photophysical parameters. An investigation of photophysical phenomena and the determination of the biosensor response pathway with biomaterials and urogenital cancer markers will provide preliminary information on proposed potential urogenital cancer biomarkers.

2. UGrants-start programme 533-K000-GS41-21,

Project duration: 01.01.2021 to 15.12.2021,
Costs: 5,000 PLN

Synthesis of hybrid materials in the form of organic dye/titanium dioxide/CNWs and titanium dioxide/CNWs thin films for alpha amino acid detection by altering electrochemical properties

d) Information on internships in national or foreign scientific or academic centres:

Internship abroad at C.N.R. Instituto di Biochimica delle Proteine, Naples, Italy from 23.20.2012 to 18.04.2013

1. Published and presented papers prior to obtaining a PhD in Physical Sciences:

a) Publications

1. **Lewkowicz, A.**; Bojarski, P.; Synak, A.; Grobelna, B.; Akopova, I.; Gryczyński, I.; Kułak, L. Concentration-Dependent Fluorescence Properties of Rhodamine 6G in Titanium Dioxide and Silicon Dioxide Nanolayers. *The Journal of Physical Chemistry C* 2012, *116* (22), 12304–12311. <https://doi.org/10.1021/jp3022562>.
2. Synak, A.; Bojarski, P.; Grobelna, B.; Kułak, L.; **Lewkowicz, A.** Determination of Local Dye Concentration in Hybrid Porous Silica Thin Films. *The Journal of Physical Chemistry C* 2013, *117* (21), 11385–11392. <https://doi.org/10.1021/jp401839j>.
3. **Lewkowicz, A.**; Synak, A.; Grobelna, B.; Bojarski, P.; Bogdanowicz, R.; Karczewski, J.; Szczodrowski, K.; Behrendt, M. Thickness and Structure Change of Titanium (IV) Oxide Thin Films Synthesized by the Sol–Gel Spin Coating Method. *Optical Materials* 2014, *36* (10), 1739–1744. <https://doi.org/10.1016/j.optmat.2014.02.033>.
4. **Lewkowicz, A.**; Synak, A.; Bojarski, P.; Grobelna, B.; Karczewski, J.; Jankowski, D.; Mahlik, S. Aggregation of Rhodamine 6G in Titanium Dioxide Nanolayers and Bulk Xerogels. *Optical Materials* 2014, *36* (10), 1694–1697. <https://doi.org/10.1016/j.optmat.2014.01.026>.
5. Pennacchio, A.; Ruggiero, G.; Staiano, M.; Piccialli, G.; Oliviero, G.; **Lewkowicz, A.**; Synak, A.; Bojarski, P.; D’Auria, S. A Surface Plasmon Resonance Based Biochip for the Detection of Patulin Toxin. *Optical Materials* 2014, *36* (10), 1670–1675. <https://doi.org/10.1016/j.optmat.2013.12.045>.
6. **Lewkowicz, A.**; Synak, A.; Grobelna, B.; Kułak, L.; Bojarski, P. Spectroscopic Properties of Rhodamine B Entrapped in Hybrid Porous Nanolayers at High Dye Concentration. *Chemical Physics* 2014, *439*, 121–127. <https://doi.org/10.1016/j.chemphys.2014.05.016>.
7. Synak, A.; Grobelna, B.; Kułak, L.; **Lewkowicz, A.**; Bojarski, P. Local Dye Concentration and Spectroscopic Properties of Monomer–Aggregate Systems in Hybrid Porous Nanolayers. *The Journal of Physical Chemistry C* 2015, *119* (25), 14419–14426. <https://doi.org/10.1021/acs.jpcc.5b03501>.

b) Presentations at scientific conferences

1. 13th International Conference on Theoretical Aspects of Catalysis, Matsushima Ichinobo w Japoni, 21.06-25.06.2010 **poster** (co-author) *DFT calculations on noble metal N-heterocyclic carbene complex for methane activation*.
2. 13th International Conference on Theoretical Aspects of Catalysis, Matsushima Ichinobo w Japoni, 21.06-25.06.2020 **poster** (co-author) *Mechanism of estrification on heteropolyacid catalyst. Theoretic DFT studies*.
3. 13th International Conference on Theoretical Aspects of Catalysis, Matsushima Ichinobo w Japoni, 21.06-25.06.2010 **poster** (co-author) *Electronic structure of the active centres in molybdenum heteropolyacids and oxide*.

4. 13th International Conference on Theoretical Aspects of Catalysis, Matsushima Ichinobo w Japoni, 21.06-25.06.2010 **oral** (co-author) *Electronic structure of model heteropolyacids and their salts. Periodic DFT study.*

5. Conference Porous Glasses-Special Glasses, PGL'2011, Wrocław, 30.08-3.09.2011- **poster** (main author), *Fluorescent properties of Rhodamine 6G in different xerogel nanolayers at high dye concentrations*

6. Conference Molecules and Light 2011, Zakopane, Poland, 19.09-24.09.2011- **poster** (main author) *Fluorescent properties of Rhodamine 6G in different xerogel nanolayers and bulk materials*

7. Conference MOLMAT 2012, Barcelona, Spain, 03-06.07.2012- **poster** (main author), *Fluorescent properties of dye-doped titanium dioxide and silica dioxide thin films for nano-optoelectronic applications*

8. Conference Krysztaly Molekularne 2012, Gdańsk-Sobieszewo, Poland 10-14.09.2012- **poster** (main author) *Właściwości fluorescencyjne rodamine 6G domieszkowanej dwutlenkiem tytanu i dwutlenkiem krzemu w postaci nanowarstw*

9. Conference IWASOM 4th, 14-19.07.2013, Gdańsk, Poland- **poster** (main author) *Properties of titanium dioxide nanolayers in the systems produced by sol-gel technique and Aggregation of Rhodamine 6G in titanium dioxide nanolayers and bulk xerogels* **oral presentation** (co-author) *Local concentration of Rhodamine 101 in nanolayers based on silica*

10. Conference PPM- Porous and Powder Materials Symposium and Exhibition, Cesme Izmir, Turkey, 3-6.09.2013- **poster** (co-author) *Synthesis, characterization and luminescence properties of xerogels doped with mixed lanthanide unguate, Spectroscopic properties of merocyanine 540 entrapped in titanium dioxide thin film, Spectroscopic properties of rhodamine B entrapped in hybrid porous nanolayers*

11. Conference IVC 2013, Paris, France 09-13.09.2013- **poster** (main author) *Fluorescence properties of merocyanine entrapped in titanium dioxide thin film*

12. Conference 1st International Caparica Conference on Chromogenic and Emissive Materials, Lisbon, Portugal, **oral presentation** (main author) *Spectroscopic properties of Rhodamine B entrapped in hybrid porous nanolayers*

2. Conferences, oral and poster presentations following the award of the Doctor of Physical Sciences degree:

1. *Analiza 3 w 1 śladu daktyloskopijnego przy użyciu spektroskopii molekularnej*, Czarnomska Martyna, **Lewkowicz Aneta**, Gruszczyńska Emilia, Bojarski Piotr, Steinborn Sławomir, 2023, XXVIII Lublin Biophysical Workshop 2023 - **oral presentation**

2. *Quick detection of drugs in fingerprints – functional tool for investigation*, Czarnomska Martyna, **Lewkowicz Aneta**, Gruszczyńska Emilia, Kasprzak Magdalena, Bojarski Piotr, Steinborn Sławomir, Woźniewski Krzysztof, Gryczyński Zygmunt, Pierpaoli Mattia, 2023, The Stockholm Criminology Symposium 2023 - **oral presentation**

3. *Zastosowanie Diamond™ Nucleic Acid Dye do analizy DNA w śladzie daktyloskopijnym*, Czarnomska Martyna, **Lewkowicz Aneta**, Gruszczyńska Emilia, Gryczyński Zygmunt,

Bojarski Piotr, Steinborn Sławomir, 2023, XIX Congress of the Polish Society of Forensic Medicine and Criminology entitled. 'New trends in human examination for forensic purposes'. 2023, **oral presentation**

4. *Aggregates of 1,8-diazafluoren-9-one – a non-toxic method for the detection of fingerprints on standard and thermal papers*, Lewkowicz Aneta, Gruszczyńska Emilia, Kasprzak Magdalena, Chabowska Michalina, Czarnomska Martyna, Walczewska-Szewc Katarzyna, Pierpaoli Mattia, Karpienko Katarzyna, Wróbel Maciej, Bogdanowicz Robert, Bojarski Piotr, Woźniewski Krzysztof, 2023, The Stockholm Criminology Symposium 2023, **oral presentation**

5. *Projektowanie molekularne w analizie śladowej*, **Lewkowicz Aneta**, Czarnomska Martyna, Gruszczyńska Emilia, Bojarski Piotr, 2023, XXVI Conference "Nowoczesne metody instrumentalne w analizie śladowej" 2023 - **oral presentation**

6. *Nowatorska, nietoksyczna metoda wizualizacji śladów daktyloskopijnych na papierach standardowych i termicznych*, Woźniewski Krzysztof, **Lewkowicz Aneta**, Kasprzak Magdalena, 2023, Forensic science convention „Forensic science - a beautiful 130-year-old" 2023, **oral presentation**

7. *Visualisation of a friction ridge using molecular spectroscopy*, Czarnomska Martyna, Gruszczyńska Emilia, **Lewkowicz Aneta**, Gryczyński Zygmunt, Bojarski Piotr, Steinborn Sławomir, 2023, 23th Annual Conference “BioInformatics in Toruń - BIT23” 2023, **poster**

8. *Revealing trace amounts of xenobiotics in the friction ridge analysis by Raman spectroscopy*, Czarnomska Martyna, **Lewkowicz Aneta**, Bojarski Piotr, Steinborn Sławomir, Woźniewski Krzysztof, 2022, 7th International Workshop on Advanced Spectroscopy and Optical Materials 2022, **poster**

9. *Spectroscopic fluorescence proofs of 1,8-diazafluoren-9-one aggregates – first reports for Friction Ridge Analysis*, Lewkowicz Aneta, Czarnomska Martyna, Kantor Małgorzata, Walczewska-Szewc Katarzyna, Bojarski Piotr, Zalewski Wojciech, Woźniewski Krzysztof, 2022, European Academy of Forensic Science Conference 2022, **poster** 10. *Spectroscopic properties of 1,8-diazafluoren-9-one in rigid media as visualization agent for friction ridge analysis*, **Lewkowicz Aneta**, Chabowska Michalina, Czarnomska Martyna, Karpienko Katarzyna, Wróbel Maciej, Sokołowski Patryk, Bojarski Piotr, Woźniewski Krzysztof, 2022, 7th International Workshop on Advanced Spectroscopy and Optical Materials 2022, **poster**

11. *AI-assisted Raman spectroscopy for characterization of vertically - oriented graphene nanostructures* 6th International Conference on Nanotechnology for Instrumentation and Measurement, 25-26.11.2021 **oral presentation (co-author)**

12. *The changes in prolyl oligopeptidase structure upon inhibition modify its ability to decrease alpha-synuclein aggregation* European Chemical Biology Symposium 2021 **oral presentation (co-author)**

13. *Ultra-sensitive luminescence characterization as a novel approach in medical sensing and fingerprint recognition* European Chemical Biology Symposium 2021 **Lewkowicz Aneta**, Pierpaoli Mattia, Bogdanowicz Robert, Zygadło Paulina, Zalewski Wojciech, 2021, European Chemical Biology Symposium 2021 - **poster**

14. *The evaluation of photophysical properties of advanced biomaterials directed on potential biomarkers of the urogenital tract cancer diseases* Workshop for Young Researchers in

Ceramics and Glasses for Medical Applications, YouCGMed, Madrid, 10.10.2019, **Aneta Lewkowicz**, Piotr Bojarski, Robert Bogdanowicz et all - **oral presentation**

15. *Surface and spectroscopic properties of 1,8-diazafluoren-9-one in titanium dioxide thin films*, International Symposium on Molecular Spectroscopy 73Rd, Champaign-Urbana, Illinois, USA, 8-22.06.2018 **Aneta Lewkowicz** - **oral presentation**

16. *Spectroscopic and structural properties of hybrid materials doped with 1,8-diazafluoren-9-one* 13th Nanosomat Conference 2018, 11-14.09.2018, Gdańsk **Aneta Lewkowicz** - **oral presentation**

17. *Charakterystyka strukturalno-spektroskopowa sondy luminescencyjnej 1,8-diazafluoren-9-onu (DFO) w matrycy stałej ditlenku tytanu*, IV Ogólnopolska Konferencja Naukowa „Fizykochemiczne badania śladów kryminalistycznych – nowoczesne technologie a opinia biegłego”, 20-23.11.2018, Bronisławów **Aneta Lewkowicz** - **oral presentation**

18. *Preparation and characterization of TiO₂/Carbon Nanowall composite on a transparent substrate*, Konferencja OPTO 2018, 4-7.07.2018, Mattia Pierpaoli, **Aneta Lewkowicz**, Maria Letizia Ruello, Robert Bogdanowicz - **poster**

19. *Spectroscopic studies of inclusion complexation between benzoic acid derivatives and α and γ cyclodextrin nanocavities*, Joint Conference Phosphor Safari and the Sixth International Workshop on Advanced Spectroscopy and Optical Materials (PS-IWASOM), Gdańsk, 9–14.07.2017, K. Baranowska, **A. Lewkowicz**, M. Józefowicz - **poster**

20. *Spectroscopic characterization of 1,8-diazafluoren-9-one as an useful fluorescent probe for urogenital tract cancer detection*, Conference Phosphor Safari and the Sixth International Workshop on Advanced Spectroscopy and Optical Materials (PS-IWASOM), Gdańsk, 9–14.07.2017, **A. Lewkowicz**, K. Baranowska, M. Józefowicz – **poster**

6. Presentation of teaching and organizational achievements as well as achievements in popularization of science or art.

6.1 Information on the didactic achievements and supervision of students as a tutor or supervisor.

I promote methods of didactic innovation and modern forms of teaching. I have the skills to activate students to work during not only exercises but also lectures. I completed **the Innovative Teaching Methods training in 2020** and the training at Ghent University (Belgium), and I subsequently obtained a Master of Didactics degree in 2022. I received the international qualification of **Master of Didactics Programme Ghent University**. My completion of postgraduate studies in **Pedagogy (2019)** and **Educational Management (2020)** at the Faculty of Educational Studies, Ateneum Academy in Gdansk, Poland, provided me with the didactic qualification to work with students at the highest possible level. My most significant contribution to the educational offer of the Faculty has been the coordination of didactic cooperation in the popularisation of physics in forensic science. I have implemented didactic reform by introducing didactic innovations within the framework of cooperation between WMFiI UG and WPiA UG. I am also involved in the process of developing the Criminology major, with particular emphasis on the Forensic Science specialisation at the Faculty of Law and Administration UG. I am a member of the Curriculum Council for the Criminology specialisation and I play an active role in the work aimed at the development of the educational process, with particular attention to the practical elements of the development of didactic cooperation with external entities, such as the Institute of Forensic Expertises in Krakow or specialists in physical and chemical analyses from forensic laboratories.

The didactic innovations I introduced are described in detail in the chapter entitled **‘Project work as a practical form of education for involving the student in the learning process’** in the book *"Educatio iuris-ars boni et aequi"*, edited by Dr. Hab. Małgorzata Balwicka-Szczyrba (2023). The overarching aim of this book is to propose a model of an exemplary university education, which is also intended to serve as a model for an effective teacher.

a) Didactic innovations applied:

The innovations I use in the education of students and pupils, involve:

- individualisation of the student
- high communicativeness during classes, innovative introduction of chat (an attempt to activate on the basis of the knowledge possessed, without substantive preparation) and substantive discussions, after prior preparation, and acquiring knowledge on a given topic in the field of physics and chemistry (as verbal methods) during lectures and demonstrations, one of the forms of educational methods stimulating reactivity to the knowledge imparted, the so-called cognitive activation of the student, formation of creative, critical individuals, characterised by a rich personality
- implementation of a pedagogical experiment for 1st grade students at the Primary School, who became students of the University of Gdansk (during the pedagogical experiment) and actively participated in lectures, demonstrations and exercises at the

Faculty of Mathematics, Physics and Computer Science: Hocus-pocus in Physics, and Working as a Forensic Technician.

- conducting lectures Revealing traces and evidence of crime - winter semester 2020 in the form of a game - using an innovative form of teaching: gamification and thinking through visualisation

b) Courses taught between 2016 and 2024:

1. Physics, 3rd year, exercises, Molecular Physics (30h)
2. Medical Physics, 4th year, exercises (30h)
3. Medical Physics I year, II level, stationary, exercises (30h)
4. Physics, 3rd year, laboratory, II Physical laboratory (23h)
5. Radiation Safety and Protection, 3rd year, full-time, Advanced Physical Laboratory (30h)
6. Quantum Information Technology 4th year, (QIT) Laboratory (23h)
7. Medical Physics, 3rd year, laboratory, Spectroscopy of biological systems (15h)
8. Criminology, specialization Forensic Science, full-time (30h) and part-time (15h)
9. lecture - full-time and part-time - Criminology MSU2 - Scientific methods of examining traces of crime by physical methods.
10. laboratory - full-time (45h) and part-time (45h) - Criminology MSU2- Scientific methods of examining traces of crime by physical methods.
11. lecture - Criminology MSU1- full-time and part-time- Revealing traces and evidence of crime by physical methods.
12. Criminology, specialization Forensic Science, 4 and 5, Master's Seminar (30h, 20h, 10h)
13. Criminology, Bachelor's Seminar (15h and 20h)

6.2 Participation in conferences, training and teaching workshops or research staff exchange programmes:

1. Participation in the 3rd Forensic Microscopy Conference, 20.10.2017
2. Participation in the Training on Modern Apparatus - Molecular Spectroscopy – Warsaw - 2017.
3. Pedagogical postgraduate studies, 26.02.2019, Ateneum Academy in Gdańsk (three semester postgraduate studies)
4. Educational management - postgraduate studies, 1.06.2020, Ateneum Academy in Gdańsk (two-semester postgraduate studies)
5. Training in innovative methods of teaching: Gamification, 15.12-16.12.2020
6. Training in innovative methods of teaching: Visual Thinking, 9.12-11.12.2020
7. VIII National Tutoring Congress: 24-26.09.2021 - training and workshops on tutoring at school and University

8. 3rd National Conference on Education and Local Government Online- EDUCATION IS COMMUNICATION 27-28.10.2021.
9. Participation in the project 'Champions of didactics - implementation of the tutoring model into university practice', Ghent University, Ghent, Belgium, Implementation of tasks within the project started in the academic year 2020/2021 (40 h) Period of realization of the subject of the contract: until 31.12.2022.
10. Participation in the project SEA EU - propose a Learning Online Course (LOC) - Physics in Forensic Science - workshops/laboratory.
11. Participation in the 'Able from Pomerania' project - 2018, 2020, 2021- series of lectures and workshops for primary and secondary school students
12. Lecture and workshop as part of the CLIMATE FOR SCIENCE - SCIENCE PICNIC AT UG 2021

6.3 Funding obtained for teaching activities (e.g. from the Teaching Initiatives Fund)

FID grant (UG Teaching Initiatives Fund) - 500/5200-S650-17- Introducing Forensic Science students to modern science research methods - contractor.

6.4 Supervising Dissertations:

My didactic activities have been honoured with numerous master's and bachelor's theses in the field of applications of physical methods in forensic science.

- **Masters: 24 (2017-2023)**
- **Bachelor's: 18 (in 2021-2023)**

Examples of thesis topics defended in 2023:

1. Analysis of the influence of substrate polarity on the disclosure of dactyloscopic traces
2. Application of delayed fluorescence phenomena in forensic investigations
3. Spectroscopic analysis of tryptophan as a potential marker for determining time of death
4. Determination of ethanol in sweat as a potential diagnostic tool useful in forensic science
5. Analysis of DNA in dactyloscopic footprints by direct PCR and horizontal gel electrophoresis using the fluorescent dye Diamond™ Nucleic Dye

I am currently supervising nine Master's theses. The theses deal with the detection of forensic traces using various physicochemical methods and physical phenomena with a special focus on the phenomenon of fluorescence and other processes of energy deactivation of excited states.

A particular development of my teaching effectiveness in the field of forensic science at our University was observed by an award at the Forum of the Polish Forensic Society in 2023, where the Master's thesis, of which I am the supervisor, was awarded.

It is noteworthy that out of such a large number of my MSc students, two have gone on to further research careers and have passed the examination for the Doctoral School in the Physical Sciences.

I am the coordinator of their laboratory work and provide scientific supervision of their experimental progress. I am the coordinator of international doctoral internships on the side of the University of Gdansk, Faculty of Mathematics, Physics and Computer Science:

Research internship of P. Martyna Czarnomska June 2023 (Doctoral School of Science and Natural Sciences UG) within the Erasmus programme at Marche Polytechnic University - Dr. Chiara Giosue (coordinator on the side of Marche Polytechnic University), Aneta Lewkowicz (coordinator of research work on the side of the University of Gdansk).

Research internship of P. Martyna Czarnomska November 2022 (Doctoral School of Natural Sciences UG) within the NAWA PROM programme at Texas Christian University, USA- Prof. Zygmunt Gryczyński (coordinator on the side of TCU), Aneta Lewkowicz (coordinator of research work on the side of UG).

6.5 Organisational achievements:

Functions performed at the University of Gdańsk:

1. Member of the Programme Council of the Criminology major (WPiA), University of Gdansk.
2. Member of the Social and Housing Commission of the University of Gdansk.
3. Member of the Psychological and Pedagogical Commission at the University of Gdansk 2021-2022.
4. Academic tutor at the Faculty of Mathematics, Physics and Informatics and the Faculty of Law and Administration, University of Gdańsk Information on science popularisation activities

6.6 Information on science popularisation activities

I have been engaged in the dissemination of scientific knowledge, delivering numerous lectures, exercises and laboratory classes for pupils of primary and secondary schools at the University of Gdańsk. These have been conducted within the framework of the Open Days of the University of Gdańsk, within the framework of the Zdolni z Pomorza programme and within the framework of the popularisation of science in the school environment.

My extensive experience of teaching, gained over many years, has been informed by my role as a scientist-researcher specialising in applied didactic methods. Furthermore, my strong commitment to self-development as a didactician, both nationally and internationally, has contributed to the advancement of higher education and the education of students to the highest didactic standards.

1. work in the field of popularisation of science, Aneta Lewkowicz: pedagogical experiment: lecture, demonstrations, exercises 'Hocus-Pokus in Physics' and Revealing fingerprint traces - for first grade students of primary school conducted at WMFiI UG - 2018, 2023.
2. participation in SEA EU project - propose a Learning Online Course (LOC) - Physics in Forensic Science -workshops/laboratory.
3. participation in the 'Gifted from Pomerania' project - 2018, 2020, 2021, 2022- series of lectures and workshops for primary and secondary school students.

4. lecture and workshops as part of CLIMATE FOR SCIENCE - SCIENCE PICNIC at UG 2021.

participation in the conference 'Gifted from Pomerania' at the Gdansk University of Technology, 'Gifted from Pomerania' in 2017, promotion of students to speak at the poster session, students of primary school No. 57 in Gdansk.

7. Additional important information concerning my career.

7.1 Scientometric data

Hirsch index: 8 (Web of Science), 8 (Google Scholar)

Total number of points of the Ministry of Education and Science for publications in the series of publications constituting the Applicant's achievement: 1180

7.2 Awards and scholarships:

- International Doctoral Projects 'Physics of future quantum-based information technologies' financed by the Foundation for Polish Science in the framework of the Innovative Economy Operational Programme - **scholarship holder, internship abroad.** 2010-2014
- **Interdisciplinary Doctoral Studies (ISD)** 'Advanced Materials for Modern Technologies and Future Energy'. - as part of the Human Capital Operational Programme, Priority IV, 'Higher Education and Science', Measure 4.1 'Strengthening and development of didactic potential of universities and increasing the number of graduates in fields of study of key importance to the knowledge-based economy' - scholarship holder 2009/2010
- **Individual award of the Rector of the University of Gdańsk**- Individual award of the second degree for scientific achievements documented by publications and creative participation in using the results of scientific work in practice in the practical application of the results of scientific work, 2023.
- **Polish Forensic Association Award** of the XXIV Edition of the Prof. Tadeusz Hanausk Competition for the Work of the Year in the category of articles and publications Warsaw, 4.12.2023: Spectroscopic Evidence of Fluorescence by 1,8-Diazafluoren-9-One Aggregates-a Prospective New Ultrasensitive Method for Fingerprint Trace Detection. Journal of Forensic Sciences 2022, 67 (4), 1468-1475