

Sesiunea de comunicări științifice ale studenților

Ediția a II-a, 2026

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10:15	Daria Stoia	Plasmonic Calligraphy on Paper Developing a Thermoplasmonic Biosensor for Cancer-Related Biomarkers
10:30	Cucuiet Vlad	Integrated SERS–Quartz Crystal Microbalance` Analysis for Enhanced Detection of DNA Viscoelasticity and Raman Signatures
10:45	Bacila Maria	Imagistică, spectroscopie și relaxometrie de Rezonanță Magnetică Nucleară în câmpuri înalte de 11.7 T pentru studiul preclinic in vivo și ex vivo a unor tumori și organe
11:00	Sesiune postere 11:00-12:30	
12:30	Botiz (Pop) Maria	Cristalizarea copolimerilor tribloc conținând poli(ϵ -caprolactonă) în filme subțiri
12:45	Madalina Maria Tudor	Light-Assisted Chloroplast-Mediated Biosynthesis of Gold Nanoparticles
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Sesiunea de comunicări științifice ale studenților

Ediția a II-a, 2026

Postere și prezentări orale

Use-case driven research: from idea to fundamental principles and to product

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Point-of-need (PON) sensors have tremendous value in diagnostics (medical and non-medical) in global health and development. Lateral flow assays are the most common PON diagnostic devices, but they lack sensitivity, multiplexing ability, and in most cases do not provide quantitative results. Specific use-cases and market needs with potential for innovation will be presented. Examples from my lab will be highlighted, where CMOS image sensors and biomaterials are used as a platform for novel biosensor development. Fundamental principles and applications will be described. These technologies will have an impact onto fields such as PON biosensors, wearable sensors, flexible electronics, and neuromorphic devices.

Plasmonic Calligraphy on Paper Developing a Thermoplasmonic Biosensor for Cancer-Related Biomarkers

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Developing rapid, reliable, and cost-effective Point-of-Care (PoC) diagnostic tools is essential for early disease detection, accessible diagnostics in resource-limited settings, and real-time monitoring outside centralized laboratories. At the same time, advancing paper-based diagnostics requires the integration of diverse sensing modalities onto a single, cost-effective substrate. In this work, we introduce ThermoPlasSens, a hybrid platform integrating gold nanoparticles of varied morphologies – nanospheres, nanorods, and nanobipyramids – functionalized with specific biorecognition elements, and immobilized *via* a precise calligraphy technique directly on a porous paper substrate. This sensor leverages thermoplasmonic heating as the primary signal detection mechanism, supported also by complementary LSPR and SERS measurements for enhanced specificity. As a proof-of-concept for platform development and optimization, polyA-polyT DNA hybridization was employed to validate sensor design and calibration, yielding reproducible multimodal responses. Moreover, the biosensor achieved successful thermoplasmonic detection of clinically relevant targets, including microRNA sequences and two cancer biomarkers, ovarian cancer-related CA125 and prostate cancer-related PSA. Our results indicate that the thermoplasmonic response (ΔT_{\max}) offers a stable and sensitive detection platform for analyte recognition under both laser and LED exposure, while LSPR and SERS measurements confirmed the specific recognition of the analyte. By combining material versatility with portable readouts, this biosensor represents a significant step forward in the development of multiplexed, paper-based plasmonic devices for real-time diagnostics applications.

Acknowledgement

This work was supported by the grant from the Ministry of Research, Innovation and Digitisation, CCCDI - UEFISCDI, project number PN-IV-P8-8.3-PM-RO-FR-2024-0144, within PNCDI IV and by the project “Plasmon mediated biology: Exploitation of plasmonics to investigate and enhance biological processes and application to biomedical issues (acronym: BioPlasmonics)” funded by European Union – NextgenerationEU and Romanian Government, under National Recovery and Resilience Plan for Romania, contract no 760037/23.05.2023, cod PNRR-C9-I8-CF-199/28.11.2022 through the Romanian Ministry of Research, Innovation and Digitalization, within Component 9, Investment I8.

Integrated SERS–Quartz Crystal Microbalance` Analysis for Enhanced Detection of DNA Viscoelasticity and Raman Signatures

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Quartz Crystal Microbalance with Dissipation (QCM-D) and Surface-Enhanced Raman Spectroscopy (SERS) are two complementary methods for studying biomolecular interactions. In this study, we introduce a synchronized SERS/QCM-D technique to investigate both the adsorbed mass and viscoelastic properties together with the spectroscopic features of short polyadenine (polyA) DNA strands, as well as their hybridization with complementary sequences. QCM-D delivers real-time measurements of mass changes and energy dissipation, while SERS provides highly sensitive detection of molecular vibrational patterns. By combining these techniques, we can directly link mechanical responses to structural and chemical changes in DNA layers. We developed the plasmonic sensor by decorating the QCM-D chip with colloidal gold nanoparticles. By tracking shifts in frequency and dissipation alongside SERS spectra, we measured both nanomechanical parameters (such as mass loading and energy dissipation) and vibrational signatures of polyA layers of different lengths (10, 15, and 20 bases). We monitored in SERS the evolution of the adenine breathing vibration (732 cm^{-1}) as a function of different polyA length. Hybridization with polyThymine (polyT) strands led to correlated changes in both QCM-D and Raman data, enabling a direct connection between mechanical alterations and molecular-level structural changes. During hybridization we observed an overall decrease in the specific adenine peak area, regardless of DNA strand length. We followed the time evolution of the adenine peak during polyT injection and observed that the hybridization dynamics is length dependent.

Overall, this work highlights the advantages of integrating SERS and QCM-D for real-time monitoring of mechanical and spectroscopic changes in nucleic acid layers. This approach provides a strong foundation for studying soft biomolecular assemblies and supports the advancement of hybrid mechanical–spectroscopic detection systems.

Acknowledgements

This work was supported by the project “Plasmon mediated biology: Exploitation of plasmonics to investigate and enhance biological processes and application to biomedical issues (acronym: BioPlasmonics)” funded by European Union – NextgenerationEU and Romanian Government, under National Recovery and Resilience Plan for Romania, contract no. 760037/23.05.2023, cod PNRR-C9-I8-CF-199/28.11.2022, through the Romanian Ministry of Research, Innovation and Digitalization, within Component 9, Investment I8.

Cristalizarea copolimerilor tribloc conținând poli(ϵ -caprolactonă) în filme subțiri

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Diversitatea și complexitatea morfologiilor cristaline reprezintă un domeniu de interes major în studiul proceselor de cristalizare, deoarece proprietățile materialelor polimerice sunt strâns corelate cu structura lor cristalină. În această lucrare a fost investigat comportamentul de cristalizare al unei serii de șase omologi ai copolimerilor tribloc poli(ϵ -caprolactonă)-b-poli(etilen adipat)-b-poli(ϵ -caprolactonă) (PCL-b-PEA-b-PCL). Masa molară a segmentului PEA a fost menținută constantă la 2500 g/mol, în timp ce masele molare ale segmentelor PCL au variat între 1000 și 10.000 g/mol. Acești copolimeri prezintă un interes deosebit pentru aplicații biomedicale datorită biodegradabilității, biocompatibilității, proprietăților mecanice favorabile și influenței structurii asupra eliberării substanțelor active.

Pentru investigarea procesului de cristalizare s-a utilizat metoda recoacerii termice (thermal annealing), prin aplicarea unor tratamente termice în intervalul 28–42 °C. Această abordare a permis evidențierea influenței condițiilor termice asupra morfologiei și gradului de cristalinitate al polimerilor. Morfologiile obținute au fost caracterizate ca structuri monocristaline, oferind posibilitatea corelării morfologiei cristalelor cu cinetica procesului de cristalizare. De asemenea, a fost analizată influența temperaturii de cristalizare, corelată cu grosimea filmului, orientarea moleculară și formarea structurilor cristaline. Totodată, au fost investigate diferențele dintre mecanismele de cristalizare ale celor șase omologi, în funcție de masa molară specifică fiecărui copolimer. Studiul urmărește evidențierea influenței parametrilor implicați în procesul de cristalizare asupra comportamentului final al materialelor polimerice.

Imagistică, spectroscopie și relaxometrie de Rezonanță Magnetică Nucleară în câmpuri înalte de 11.7 T pentru studiul preclinic *in vivo* și *ex vivo* a unor tumori și organe

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Investigațiile preclinice privind rezonanța magnetică (RM) au devenit mai informative decât simpla achiziție a unei imagini RM calitative. În acest sens, spectroscopia RM *in vivo* și *ex vivo* și relaxometria pot oferi informații cantitative despre structura și dinamica țesuturilor și organelor biologice. În special, identificarea și caracterizarea țesuturilor tumorale sunt de mare importanță. Un tip de tumoare B16-F10 a fost crescut aproape de coloana vertebrală a unui șoarece de laborator, timp de 7 zile, apoi investigat *in vivo*. Ulterior, investigarea *ex vivo* a organelor (tumoare, creier și ficat de șoarece) fixate în formol a fost efectuată la intervale regulate de timp până la câteva luni. Acestea au presupus imagistică RM ponderată și spectroscopie RMN localizată la ¹H (cu protocol saturat în apă) și relaxometrie bazată pe RMN. Pentru aceasta, a fost măsurată o serie de 64 de "echouri" descrescătoare prin metoda CPMG, iar distribuția corespunzătoare a fost obținută prin transformata inversă Laplace. Au fost identificate două picuri (țesut tumoral *in vivo*) sau trei (țesut sănătos *in vivo*) rezolvate în distribuția . Așa cum era de așteptat, variația mare prezintă distribuția *ex vivo* a timpului de relaxare transversală, . S-a observat o ușoară deplasare către valori mici ale odată cu creșterea timpului de fixare în formol. Spectrele RMN *in vivo* ¹H ale tumorilor (și țesutului sănătos) sunt mai bogate în informații comparativ cu spectrele corespunzătoare înregistrate pentru organele formolizate. În plus, a fost obținută o serie de hărți parametrice folosite pentru caracterizarea *in vivo* și *ex vivo* a organelor de șoarece (creier și ficat) și a țesuturilor (cu tumori și sănătoase). Tehnici avansate de RMN aplicate în câmp înalt (11.75 T), cum ar fi imagistica, spectroscopia Fourier și Laplace și hărțile parametrilor , s-au dovedit a fi instrumente importante pentru caracterizarea țesuturilor tumorale, precum și pentru evaluarea efectului fixării în formol.

Digital SERS: optimisation of the quantitative chemical analysis protocol at ultra-low concentrations

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Single molecule surface-enhanced Raman spectroscopy (SM-SERS) has the potential to revolutionize quantitative analysis at ultralow concentrations (less than 1 nM) [1]. However, both quantitative and qualitative analyses remain challenging due to the low abundance of the analyte in solution and significant signal fluctuations.

As a solution to these issues, we propose a digital analysis protocol for surface-enhanced Raman scattering (SERS), which involves the acquisition of multiple short-time spectral measurements rather than long acquisitions that average the molecular signal, as is typically done in conventional SERS techniques. In the latter case, the weak spectral information is lost in averaging, whereas the signals from molecules present in high concentrations dominate the spectrum.

In this study, we highlight that the key factor for detecting low concentrations of molecules is not the intensity of the SERS band, but rather the frequency of its occurrence across multiple flash acquisitions. If a flash acquisition corresponds to the analyte spectrum, it is classified as a “positive” spectrum and assigned a value of “1”; otherwise, it is classified as a negative spectrum and assigned a value of “0” [2]. Sets of 500 spectra were acquired at several ultra-low analyte concentrations, and the corresponding number of positive spectra was determined. A linear calibration curve relating analyte concentration to the number of occurrences was then constructed.

Once established, this calibration enables the determination of the analyte concentration in an unknown sample by counting the number of positive spectra within a set of 500 acquisitions. We optimized the identification of positive spectra using multiple approaches, including scalar product comparison with a high-concentration reference spectrum, and principal component analysis. After identifying the optimal method for determining the number of occurrences, we applied it to two different substrates, liquid and solid, to assess in which case the calibration curve performs better and we demonstrated that the liquid substrate is more efficient.

References

- [1] C. D. L. de Albuquerque, R. G. Sobral-Filho, R. J. Poppi, and A. G. Brolo, *Anal. Chem.*, vol. 90, no. 2, pp. 1248–1254, Jan. 2018
- [2] X. Bi, D. M. Czajkowsky, Z. Shao, and J. Ye, *Nature*, vol. 628, no. 8009, pp. 771–775, Apr. 2024

Light-Assisted Chloroplast-Mediated Biosynthesis of Gold Nanoparticles

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Gold nanoparticles (AuNPs) exhibit size-dependent optical properties that make them attractive for light-driven biohybrid applications. In this context, this work investigates chloroplast-mediated AuNP biosynthesis as a green, light-assisted strategy for producing biocompatible AuNPs and understanding the role of chloroplast-derived components in Au³⁺ reduction. Chloroplasts isolated from *Spinacia oleracea* were first characterized by UV-Vis absorption, circular dichroism, and fluorescence spectroscopy to assess pigment organization and integrity. The biosynthesis of AuNPs was then carried out under 455 nm LED irradiation, chosen to match the blue absorption region of chloroplast pigments and promote resonant photoactivation. Two systems were compared: intact chloroplast suspensions and the supernatant obtained after washing damaged chloroplasts. AuNPs formation was confirmed by UV-Vis spectroscopy through LSPR bands at 547 nm and 537 nm, respectively, while TEM revealed average diameters of 19.8 ± 3.4 nm and 6.9 ± 2.6 nm. Additionally, real-time thermal monitoring, circular dichroism before and after irradiation, and Fluorescence Lifetime Imaging Microscopy were used to elucidate the mechanisms governing AuNPs formation and AuNPs-chloroplast interactions. Overall, both systems mediated AuNPs formation under resonant blue-light irradiation, but produced nanoparticles with distinct optical and size characteristics. These results suggest that intact chloroplast structure and released biomolecular components contribute differently to Au³⁺ photoreduction, nanoparticle growth, and colloidal stabilization, supporting chloroplast-based nanosystems as promising platforms for bioinspired plasmonic nanomaterial synthesis.

Acknowledgements

This work was supported by the project “Plasmon mediated biology: Exploitation of plasmonics to investigate and enhance biological processes and application to biomedical issues (acronym: BioPlasmonics)” funded by European Union – NextGenerationEU and Romanian Government, under National Recovery and Resilience Plan for Romania, contract no 760037/23.05.2023, cod PNRR-C9-I8-CF-199/28.11.2022, through the Romanian Ministry of Research, Innovation and Digitalization, within Component 9, Investment I8.

Periodic solutions of nonlinear fractional diffusion equations

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We study the existence of time-periodic mild solutions for nonlinear fractional diffusion equations with exterior Dirichlet condition on a bounded domain. The diffusion is generated by the constrained fractional Laplacian $(-\Delta)^s$, $s \in (0, 1)$, together with a linear damping term λu , and the analysis is carried out in the Hilbert space $L^2(\Omega)$. We first formulate the problem as an abstract semilinear evolution equation governed by the family of operators $A_s + \lambda I$. Using Mosco convergence of the associated energy forms, we prove strong resolvent convergence and, consequently, strong convergence of the corresponding semigroups, locally uniformly with respect to time, as s varies in $[0, 1]$. This yields continuity of mild solutions with respect to the fractional parameter. Finally, combining compactness of the translation along trajectories operator with the Leray–Schauder degree, we establish the existence of T -periodic mild solutions for $s \in (0, 1]$ under growth and dissipativity assumptions on the Nemytskii operator. The degenerate endpoint $s = 0$ is included in the convergence analysis and is discussed separately, since the limiting semigroup is not compact on $L^2(\Omega)$.

Bibliografie

- [1] C. O. Alves, F. J. S. A. Corrêa, On the existence of periodic solutions for semilinear evolution equations with noncompact semigroups, *J. Differential Equations* 163 (2000), no. 1, 116–131.
- [2] J. Bourgain, H. Brezis, P. Mironescu, Another look at Sobolev spaces, *Optimal Control and Partial Differential Equations*, IOS Press, Amsterdam (2001), pp. 439–455.
- [3] H. Brezis, *Functional Analysis, Sobolev Spaces and Partial Differential Equations*, Universitext, Springer, 2011.
- [4] L. Caffarelli, L. Silvestre, An extension problem related to the fractional Laplacian, *Comm. Partial Differential Equations* 32 (2007), no. 7–9, 1245–1260.
- [5] T. Cazenave, *Semilinear Schrödinger Equations*, Courant Lecture Notes in Mathematics, vol. 10, Courant Institute of Mathematical Sciences, New York, 2003.
- [6] T. Cazenave, A. Haraux, *An Introduction to Semilinear Evolution Equations*, revised edition, Clarendon Press, Oxford, 1998.
- [7] K. Deimling, *Nonlinear Functional Analysis*, Springer-Verlag, Berlin, 1985.
- [8] E. Di Nezza, G. Palatucci, E. Valdinoci, Hitchhiker's guide to the fractional Sobolev spaces, *Bull. Sci. Math.* 136 (2012), no. 5, 521–573.
- [9] T. Kato, *Perturbation Theory for Linear Operators*, second edition, Springer-Verlag, Berlin-New York, 1976.
- [10] U. Mosco, Composite media and asymptotic Dirichlet forms, *J. Funct. Anal.* 123 (1994), no. 2, 368–421.
- [11] A. Pazy, *Semigroups of Linear Operators and Applications to Partial Differential Equations*, Springer-Verlag, New York, 1983.
- [12] M. Reed, B. Simon, *Methods of Modern Mathematical Physics. I. Functional Analysis*, Academic Press, New York-London, 1972.
- [13] R. Servadei, E. Valdinoci, On the spectrum of two different fractional operators, *Proc. Roy. Soc. Edinburgh Sect. A* 144 (2014), no. 4, 831–855.

Gold Nanoparticles for Modulating Oxygen Evolution in Chloroplast-Based Artificial Photosynthesis Systems

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Artificial photosynthesis aims to develop systems capable of efficiently harvesting solar energy and storing it in the form of chemical bonds. These systems typically combine a light-absorbing component with a catalyst that promotes charge-transfer processes. In this context, bovine serum albumin-functionalized gold nanoparticles (AuNPs@BSA), designed to improve colloidal stability and biocompatibility, were investigated as plasmonic nanostructures in a biomimetic artificial photosynthesis system based on chloroplasts isolated from spinach. Chloroplasts were isolated and characterized by UV-Vis spectroscopy to assess pigment integrity and optical response. The aim of this work was to investigate dissolved oxygen dynamics in chloroplast -AuNPs hybrid systems under plasmonic excitation. Photosynthetic activity was assessed by monitoring dissolved oxygen over time using an oxygen sensor, both in the dark and under LED irradiation at 530 nm, corresponding to the localized surface plasmon resonance band of the designed AuNPs. The results show that AuNPs@BSA significantly influence dissolved oxygen dynamics, suggesting plasmon-mediated effects on charge-transfer processes, potentially involving hot electrons. The effect of LED intensity was also examined, showing that excessive irradiation can damage chloroplasts and disrupt photosynthetic activity. Overall, this study highlights the potential of AuNPs@BSA to modulate oxygen-related photochemical processes in chloroplast-based artificial photosynthesis systems.

Acknowledgements

This work was supported by the project “Plasmon mediated biology: Exploitation of plasmonics to investigate and enhance biological processes and application to biomedical issues (acronym: BioPlasmonics)” funded by European Union – NextgenerationEU and Romanian Government, under National Recovery and Resilience Plan for Romania, contract no 760037/23.05.2023, cod PNRR-C9-I8-CF-199/28.11.2022, through the Romanian Ministry of Research, Innovation and Digitalization, within Component 9, Investment I8.

Plasmon-Assisted Photocatalysis on Tunable Au-Ag Core-Shell Nanorods: Insights into the Hot-Hole Driven Conversion of pATP to DMAB

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Plasmonic core-shell nanoparticles provide tunable optical properties that make them attractive platforms for photocatalytic and Surface Enhanced Raman Spectroscopy (SERS)-based applications, as their optical response can be tuned through both core composition and shell growth. In this study, Au-Ag core-shell nanorods were synthesized through a two-step approach, consisting of gold nanorod preparation followed by controlled silver shell growth. The synthesis was optimized by varying the volumes of AgNO₃, NaOH, and CTAB to control shell formation, colloidal stability, and plasmonic response. The optimized nanoparticles were functionalized with p-aminothiophenol (pATP), used as a model molecule to investigate the plasmon-mediated conversion to 4,4-dimercaptoazobenzene (DMAB), monitored by SERS. Catalytic efficiency was evaluated as a function of irradiation wavelength, pH, and temperature, under resonant (532 and 638 nm) and non-resonant (808 and 980 nm) excitation conditions. The influence of pH was investigated in the 5-11 range, showing enhanced photocatalytic efficiency under alkaline conditions, followed by a plateau at higher pH values. Temperature-dependent measurements were used to evaluate thermal contributions, while hydrogen peroxide and methanol experiments were performed to elucidate the involvement of plasmon-generated charge carriers, particularly hot holes, in the reaction mechanism. Overall, this study highlights the potential of Au-Ag core-shell nanorods as tunable plasmonic platforms for SERS-monitored photocatalytic and hot-carrier driven processes.

Acknowledgments

This work was supported by the project “Plasmon mediated biology: Exploitation of plasmonics to investigate and enhance biological processes and application to biomedical issues (acronym: BioPlasmonics)” funded by European Union – Nextgeneration EU and Romanian Government, under National Recovery and Resilience Plan for Romania, contract no 760037/23.05.2023, cod PNRR-C9-I8-CF-199/28.11.2022, through the Romanian Ministry of Research, Innovation and Digitalization, within Component 9, Investment I8.

Stochastic Pricing of Derivative Financial Instruments

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Option pricing and trading play an important role in modern financial markets, particularly in the context of risk management. This project develops a numerical application for evaluating the price of American-style stock options based on the Least Squares Monte Carlo algorithm. Three models for the simulation of the underlying asset evolution are compared: Geometric Brownian Motion, Heston Stochastic Volatility, and Merton Jump-Diffusion. The calculated option prices are tested against historical market data for SPY, QQQ, and AAPL options using two trading strategies: statistical arbitrage and delta-hedging. Across all tests, a favorable profit evolution is obtained, indicating good accuracy of the pricing models. Stochastic Volatility proves to be a better fit for arbitraging individual stocks, while Geometric Brownian Motion offers a better balance between precision and computational cost for exchange-traded funds. In the context of delta-hedging, the models' profitability is similar, with Geometric Brownian Motion again leading in terms of computational efficiency. These results provide a foundation for the development of more advanced option pricing and trading models, relevant especially for market making applications.

TREE-BASED MACHINE LEARNING MODEL FOR FLUORESCENCE LIFETIME PREDICTION IN ORGANIC COMPOUNDS

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Fluorescence lifetime is a fundamental excited-state property describing the average time a fluorophore remains in the excited state before photon emission. It reflects the competition between radiative and non-radiative decay pathways and is therefore important for fluorescence lifetime imaging microscopy, sensing, optoelectronic materials and high-throughput fluorophore screening [1]. However, experimental lifetime measurements require specialized instrumentation, while time-dependent density functional theory can be computationally demanding for large molecular libraries.

This study presents an interpretable tree-based machine learning framework for predicting fluorescence lifetimes of organic chromophores in solvent environments. The model was developed using chromophore-solvent data derived from the Deep4Chem database [2]. Molecular structures were represented using RDKit descriptors, Morgan and MACCS fingerprints, three-dimensional geometry descriptors, predicted pKa values and engineered photophysical features, including absorption/emission descriptors, and chromophore-solvent interaction terms. A LightGBM regressor [3] was selected because it provides efficient learning and strong interpretability for heterogeneous tabular molecular descriptors.

The optimized model was evaluated using cluster-stratified cross-validation and achieved a mean absolute error of 0.8324 +/- 0.0617 ns and an R2 value of 0.7523 +/- 0.0317. External validation against TD-DFT benchmark systems and independent experimental data confirmed that the model captures global lifetime trends and can support rapid screening. SHAP analysis [4] identified quantum yield, molecular geometry, emission-related descriptors, topological indices and local fragment motifs as key contributors, indicating that the model learns physically meaningful structure-property relationships. Overall, this workflow provides a fast and interpretable route for fluorescence lifetime prediction and fluorophore prioritization.

Keywords: Fluorescence lifetime; Machine learning; LightGBM; Chromophores; Molecular descriptors

References

- [1] J. R. Lakowicz, Principles of Fluorescence Spectroscopy, 3rd ed.; Springer, Boston, MA, 2006.
- [2] J. F. Joung, M. Han, M. Jeong, S. Park, Sci. Data 7, (2020) 295.
- [3] G. Ke, Q. Meng, T. Finley, T. Wang, W. Chen, W. Ma, Q. Ye, T.-Y. Liu, Adv. Neural Inf. Process. Syst. 30, (2017).
- [4] S. M. Lundberg, S.-I. Lee, Advances in Neural Information Processing Systems 30, (2017) 4765–4774.

Simulation-Guided Optimization of Ordered Nanosphere Lithography Plasmonic Substrates for Ultrasensitive SERS Detection

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Plasmonic nanobiosensors have emerged as powerful tools for molecular diagnostics by enabling label-free and highly sensitive detection through Surface-Enhanced Raman Scattering (SERS). This study presents an ordered Au-NSL-Au plasmonic architecture featuring a primary gold base layer overlaid with a hexagonally ordered array of gold nanoprisms. These structures were patterned via nanosphere lithography using polystyrene spheres and were subsequently topped with a second layer of gold, the thickness of which defines the final height of the nanostructures. The architecture was designed to promote strong electromagnetic field localization and tunable plasmonic coupling for ultrasensitive SERS detection.

Initial experimental validation was conducted on an Au(30 nm)-NSL-Au(30 nm) configuration, featuring a 30 nm gold base and a subsequent 30 nm deposition to define the nanostructure height. This architecture demonstrated remarkable sensing performance, achieving a Limit of Detection (LOD) of 10⁻⁸M for the 4-mercaptobenzoic acid (4-MBA) reporter molecule. To optimize sensing performance, extensive Finite Difference Time Domain (FDTD) simulations were conducted to identify the optimal geometric parameters, namely: basal gold thickness and nanostructure height.

The study reveals that the optimal architecture is highly dependent on the excitation wavelength. For 638 nm excitation, the maximum enhancement occurs with a 40 nm basal layer and a 50 nm structure height. In contrast, for 785 nm excitation, the ideal configuration shifts to a thinner 10 nm basal layer with the same 50 nm height. These findings underline the critical role of the basal gold layer in tuning plasmonic coupling, providing design guidelines for wavelength-specific ultrasensitive SERS substrates.

Development and Characterization of Alginate-Collagen Biomaterials for Soft Tissue Regeneration

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One of the main objectives of tissue engineering is to develop biomaterials that provide an optimal environment for tissue regeneration [1]. In this study, we propose developing biomaterials based on alginate and collagen for use in regeneration of soft tissue. Alginate is a polysaccharide extracted from brown algae, characterized by low toxicity and high biocompatibility, as well as antimicrobial activity. Collagen is the most abundant protein in the human body exhibiting high biocompatibility and bioactivity, although it presents low mechanical strength [2].

Three types of alginate-collagen samples with different collagen concentrations were developed: (i.e., 95:5, 90:10, and 80:20). The materials were obtained through ionic crosslinking (Ca^{2+}) and were subjected to two cycles of freezing and lyophilization, with a duration of 24 h each. The samples were analyzed using Raman spectroscopy, Fourier Transformed Infrared Spectroscopy (FT-IR), X-ray Diffraction (XRD), Scanning Electron Microscopy (SEM), and compression testing. FT-IR data confirmed the crosslinking of the two biopolymer components. SEM analysis revealed the macroporous structure of the composite materials, with pore diameters ranging from 57 to 88 μm . Bioactivity of the composites was assessed after immersion in SBF through FT-IR, XRD and SEM analyses. The results confirmed the formation of an apatitic-like phase on the surface of the biomaterials, result that indicates their bioactivity [3]. The compressive elastic modulus showed a decreasing tendency with increasing collagen concentration, while the stiffness values remained comparable to those of the outer layer of skin.

The obtained results demonstrate the potential of the prepared scaffolds to be used as biomaterial matrices in future tissue engineering applications.

References:

- [1] Preeti Sharma, Pradeep Kumar, Rachna Sharma, Vijaya Dhar Bhatt, and PS Dhot, „Tissue Engineering; Current Status & Futursitic Scope”, *Journal of Medicine and Life*, 12, 225–229, 2019.
- [2] Leilei Sun, Yanyan Shen, Mingbo Li, Qiuting Wang, Ruimin Li, Shunmin Gong, „Preparation and Modification of Collagen/Sodium Alginate-Based Biomedical Materials and Their Characteristics”, *Polymers*, 16, 2024.
- [3] Alexandra Feraru, Zsejke-Reka Toth, Klara Magyari, Monica Baia, Tamas Gyulavari, Eموke Pall, Emilia Licarete, Codruț Costinaș, Oana Cadar, Ionel Papuc, Lucian Baia, „The effect of nanoceria on the alginate-gum arabic crosslinking mechanism and in vitro behavior as a wound dressing”, *International Journal of Biological Macromolecules*, 288, 2024.

Protein Corona Stability on Gold Nanoparticles: Structural and Photothermal Characterization under Environmental Stress

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Gold nanoparticles (AuNPs) have attracted significant interest due to their plasmonic properties, colloidal stability, biocompatibility and surface versatility, which make them highly valuable for the development of new platforms in biological applications. In this context, understanding the behavior of nano-bio interfaces, especially how protein corona interacts with the surface of AuNPs under different conditions, is essential for their effective integration into therapeutic and diagnostic systems. The present study focuses on the investigation of structural evolution of Bovine Serum Albumin (BSA) when adsorbed on AuNPs surface under varying pH and temperature conditions. The characterization was performed optically *via* UV-Vis-NIR spectroscopy, Dynamic Light Scattering and Zeta Potential measurements, while Transmission Electron Microscopy was used to characterize the morphology of the complex. In addition, the behavior of the BSA protein corona was further analyzed using advanced spectroscopic methods such as Fluorescence Emission spectroscopy and Circular Dichroism, in order to assess its thermal stability and to study its secondary structure. Moreover, photothermal studies were performed using a 532 nm laser and a 530 nm LED irradiation source that further demonstrated the protein corona protection against photo-induced destabilization, ensuring a reproducible thermal response. Overall, the results demonstrate that the protein corona not only stabilizes the AuNPs, but also actively modulates their optical and thermal properties. Such systems hold significant potential for the design of nano– bio platforms with applications in biosensing, drug delivery, and nanomedicine.

Acknowledgements

Catalina Rusu acknowledges the financial support provided by the World Federation of Scientists scholarship. Daria Stoia would like to acknowledge the financial support provided by the French government, through the UCAJEDI “Investissements d’Avenir” project, managed by the National Research Agency, ANR-15-IDEX-01.

Plasmon-Enhanced Detection of PolyA–PolyT DNA Hybridization through Chiroptical and SERS Signatures

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DNA hybridization is a fundamental biological process and an important model for studying molecular recognition and assembly mechanisms. Despite growing interest in DNA-mediated plasmonic systems, studies on DNA hybridization-driven plasmonic coupling and its associated optical and chiroptical responses remain limited. In this work, DNA-functionalized gold nanoparticles (NPs) were employed as plasmonic platforms to investigate hybridization-induced optical coupling, chiroptical activity and Surface-enhanced Raman spectroscopy (SERS) detection of the nucleobases.

Gold nanorods (AuNRs) and gold nanospheres (AuNSs) were synthesized through seed-mediated growth and the Turkevich method, respectively, and characterized by spectroscopic techniques and transmission electron microscopy (TEM). Separate AuNRs and AuNSs populations were functionalized with thiolated PolyA-SH (PolyAdenine) and PolyT-SH (PolyThymine) oligonucleotides (20 bases), previously incubated with TCEP, a reducing agent used to break disulfide bonds and protect thiolated DNA oligomers, in order to promote Au-S binding. Upon mixing the complementary DNA-functionalized NPs, PolyA-PolyT hybridization induced NP assembly and plasmonic coupling. The as-formed hybridized systems were investigated using absorption spectroscopy, SERS, and circular dichroism (CD) to evaluate the coupling efficiency and induced chiroptical responses in spherical and anisotropic NPs systems.

SERS measurements confirmed DNA hybridization through characteristic adenine vibrational signatures at $\sim 730\text{ cm}^{-1}$ and $\sim 1300\text{ cm}^{-1}$, while CD analysis revealed pronounced induced plasmonic chirality in AuNRs assemblies, particularly within the longitudinal plasmon resonance region, indicating strong coupling between hybridized DNA structures and anisotropic plasmonic NPs. These findings highlight the potential of DNA-functionalized gold NPs as plasmonic and chiroptical platforms for hybridization interactions studies.

MORPHOLOGY-DRIVEN PLASMONIC CHIRALITY IN GOLD NANOFLOWERS FOR ENANTIOSELECTIVE SENSING

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Chirality at the nanoscale enables unique plasmon–light interactions, generating distinct optical responses toward left- and right-circularly polarized light. Consequently, chiral plasmonic nanostructures are therefore attractive for enantioselective sensing and biological applications, where selective recognition of molecular enantiomers remains challenging [1]. In this context, gold nanoparticles (GNPs) with flower-like chiral morphologies were synthesized via a wet-chemical approach and evaluated as plasmonic nanoplatfoms for enantiomer discrimination. The nanoparticles, with average dimensions of approximately 195 ± 30 nm, were characterized by Transmission Electron Microscopy (TEM), zeta potential analysis, UV-Vis-NIR spectroscopy, Energy-Dispersive X-ray Spectroscopy (EDX), and Circular Dichroism (CD) spectroscopy. CD measurements confirmed the plasmonic chirality of the nanostructures through differential absorption of circularly polarized light. The flower-like GNPs exhibited a predominantly left-handed chiroptical response and demonstrated enantioselective interactions toward Tryptophan enantiomers, selected as model chiral analytes. Enantiomeric excess studies further highlighted the potential of these chiral plasmonic nanoparticles as nanoscale platforms for enantioselective sensing applications.

Keywords: Plasmonic Chirality; Circular Dichroism; Gold Nanoparticles; Enantioselectivity

References

[1] Wenbing Wu, Matthias Pauly, *Material Advances* 3, (2022) 186-215.

Structural, Magnetic and Micromagnetic Properties of $\text{Dy}_{1-x}\text{Gd}_x\text{Co}_3$ as a Candidate for Hosting Ferrimagnetic Skyrmions

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One of the most recent challenges in spintronics is the device implementation of topological magnetic textures such as magnetic skyrmions. Within this context, our study covers the area of ferrimagnetic Rare-Earth – Transition-Metal (RE-TM) alloys in structural configurations providing tuneable ferrimagnetism. The focus of the study is the ferrimagnetic intermetallic $\text{Dy}_{1-x}\text{Gd}_x\text{Co}_3$ system for which the bulk structural and magnetic properties were investigated for x ranging from 0 to 1. The samples were prepared by arc-melting under an argon atmosphere and annealed. X-ray diffraction analysis confirmed the expected structural properties of the systems. The main magnetic properties were determined through vibrating sample magnetometry. Thin films of the parent compound were deposited by Ultra-High-Vacuum magnetron sputtering and characterized via atomic force microscopy, magnetic force microscopy and Superconducting Quantum Interference Device (SQUID) magnetometry. Performing DFT calculations and comparing them to the experimental results, we confirm the ferrimagnetic order of our compounds. Furthermore, using the experimental magnetic parameters, we performed micromagnetic simulations based on the dynamic Landau-Lifshitz-Gilbert equation. These simulations indicate the parameter range in which the skyrmions can be stabilized in our materials, revealing its potential for classic and quantum skyrmionic applications.

Dezvăluirea structurii ascunse a derivaților de lawsonă prin spectroscopie RMN în stare solidă

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Lucrarea prezintă caracterizarea structurală a derivaților de lawsonă LW01-LW06 prin spectroscopie de Rezonanță Magnetică Nucleară în stare solidă. Investigația urmărește identificarea mediilor chimice locale ale nucleelor de ^1H și ^{13}C și evidențierea modificărilor structurale determinate de substituenții introduși în nucleul de lawsonă.

Analiza spectrelor ^1H MAS a permis observarea semnalelor atribuite protonilor alifatici și aromatici, confirmând prezența fragmentelor structurale caracteristice derivaților analizați. Spectrele ^{13}C CP-MAS au evidențiat semnale specifice carbonilor alifatici, aromatici și carbonilici, relevante pentru confirmarea sistemului naftochinonic.

Variațiile deplasărilor chimice dintre compuși indică modificări ale mediului electronic local, determinate de natura substituenților, fără alterarea structurii fundamentale a lawsonelor. Rezultatele obținute confirmă conservarea nucleului naftochinonic în seria LW01-LW06 și demonstrează relevanța spectroscopiei RMN în stare solidă pentru caracterizarea structurală a compușilor organici solizi.