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Bogumił Cieniek
Ireneusz Stefaniuk

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CONFERENCE PROGRAMME

MONDAY (06 / 29)

03:00 PM–05:00 PM – Registration (Pigonia Street 1, Building A0)
03:00 PM–05:00 PM – Laboratory tour
05:00 PM–07:00 PM – Welcome Reception (cold buffet, coffee, tea)

TUESDAY (06 / 30)

9:00 AM–9:15 AM – Opening Ceremony
9:15 AM–11:45 AM – Session 1 Chairman: Prof. dr hab. Czeslaw Rudowicz, UAM
  9:15 AM–10:00 AM
  Yatramohan Jana – *Electron Paramagnetic Resonance of Transition-Metal Activators in Luminescent Oxides – Case Study: Mn^{4+} Ions* [Plenary lecture]
  10:00 AM–10:35 AM
  Maria Augustyniak-Jabłokow – *EMR studies of Magnetic Defects Generated by Grinding Glass-like Carbons* [Invited lecture]
  10:35 AM–10:55 AM
  Ryhor Fedaruk – *Rabi Oscillations of Paramagnetic Centers with Short Relaxation Times: Peculiarities of Observation and Simulation*
  10:55 AM–11:45 AM
  Zbigniew Sojka – *Binding and Activation of Selected Small Molecules on Metallozeolites – Spectroscopic and DFT Insights* [Plenary lecture]
11:45 AM–12:15 PM – Coffee break
12:15 PM–1:00 PM – PG EMR General Meeting
1:00 PM–2:00 PM – Lunch
2:00 PM–5:30 PM – Excursion (to Łańcut Castle)
6:00 PM – Barbecue dinner (Sabatini Restaurant, Al. Piłsudskiego Street 17)

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  Czesław Rudowicz – *Importance of Tesseral and Spherical Tensor Operators for Describing Low-Symmetry Aspects in EMR and Optical Spectroscopy* [Plenary lecture]
  9:45 AM–10:20 AM
  Michal Zalibera – *Metal vs Ligand Control of Spin in Cu/Ni Bisamidrazones* [Invited lecture]
  10:20 AM–10:40 AM
  Danuta Piwowarska – *EPR Study of APTES/TiO_2 Nanomaterials with Temperature-Dependent Properties*
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11:10 AM–1:00 PM – Session 3 Chairman: Prof. dr hab. Maria Augustyniak-Jabłokow, PAN

11:10 AM–11:55 AM

Muhammed Açıkgöz - *A Quantitatively Constrained Framework for Defect Identification in Materials via Integrated Machine Learning, Zero-field Field Splitting Modeling, and EPR data* [Plenary lecture]

11:55 AM–12:30 PM

Bohdan Padlyak – *EPR Spectroscopy of Radiation-Induced Centers in Borate Crystals and Glasses* [Invited lecture]

12:30 PM–12:50 PM

Grzegorz Leniec – *Decoding Broadband NIR Luminescence through EPR in Cr^{3+} -Activated Mixed Spinels*

1:00 PM–2:30 PM – Lunch

2:30 PM–4:00 PM – Session 4 Chairman: dr hab. Bohdan Padlyak, LNU

2:30 PM–3:05 PM

Tomasz Czechowski – *New functionalities in multiharmonic analysis* [Invited lecture]

3:05 PM–3:40 PM

Anna Tomaszewska – *Synthesis and EPR study of the ultrasmall $Zn_{1-x}Mn_xFe_2O_4$ ferrite particles* [Invited lecture]

3:40 PM–4:00 PM

Ihor Virt – *EMR characterization of high-concentration Co/Cr-doped ZnO films on quartz and sapphire*

4:00 PM-4:30 PM – Coffee break

4:30 PM-6:00 PM – Poster session

7:00 PM – Gala dinner (Konfitura Restaurant, ul. Słowackiego 8)

THURSDAY (07 / 02)

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9:00 AM–9:35 AM

Ireneusz Stefaniuk – *EPR studies of environmentally persistent free radicals and metal ions in various fractions of airborne dust* [Invited lecture]

9:35 AM–10:10 AM

Krzysztof Kruczała – *Hydroxyl Radical Scavenging by Metal Oxide Nanoparticle Catalysts for Enhanced Stability of Alkaline Fuel Cells* [Invited lecture]

10:10 AM–10:30 AM

Kamila Sobańska – *EPR insight into the role of H_2O_2-derived ROS in the degradation of model water pollutants*

10:30 AM–10:50 AM

Wiktor Czerwonka – *Applications of EPR spectroscopy in the analysis of ROS quenchers in Fenton-type reactions*

10:50 AM–11:20 PM – Coffee break

11:20 AM–12:30 PM – Session 6 Chairman: dr hab. Ireneusz Stefaniuk, Prof. UR

11:20 AM–11:40 AM

Volodymyr Popovych – *Study of electron magnetic resonance in heavily Cr-implanted CdTe single crystals with dopant-related secondary phases*

11:40 AM–12:00 AM

Marian Kuźma – *Two-dimensional ferromagnetism in* Cr_3Te_4

12:00 AM–12:20 AM

Piotr Pisiak – *Temperature-Dependent EPR Study of Powder Coatings*

12:20 PM–12:30 PM – Closing Ceremony

12:30 PM–14:00 PM – Lunch

LECTURES

(in alphabetical order)

A Quantitatively Constrained Framework for Defect Identification in Materials via Integrated Machine Learning, Zero-field Field Splitting Modeling, and EPR data

Muhammed Açıkgöz [a]

[a] *Department of Science, State University of New York, Maritime College, New York 10465, USA*
macikgoz@sunymaritime.edu

Key words: Defect chemistry, Transition-metal doping (3dN, 4fN), Charge compensation mechanisms, Structure–property relationships, Machine learning interatomic potential (MLIPs)

Identifying the microscopic nature of defects in crystalline materials remains a central challenge in electron paramagnetic resonance (EPR) spectroscopy, particularly when competing defect configurations exhibit similar spectroscopic signatures. This work presents a quantitatively constrained computational framework for defect identification that integrates machine learning-based structural optimization, crystal field modeling, and EPR parameter analysis.

The workflow begins by generating and optimizing candidate defect structures using the CHGNet [1] machine learning interatomic potential [2,3,4], allowing efficient exploration of local structural relaxations beyond ideal crystallographic models. For each optimized configuration, zero-field splitting parameters (ZFSPs) are computed via the superposition model (SPM) [5,6] to establish a direct link between local coordination geometry and spin Hamiltonian parameters. Concurrently, bond valence sum (BVS) analysis evaluates local charge states to ensure chemical consistency.

A key feature of this framework is the simultaneous application of structural, electrostatic, and spectroscopic constraints. Calculated ZFSPs are systematically compared with experimental EPR data, and candidate defect models are refined through SPM-based fitting to achieve optimal agreement with observed parameters. As recently demonstrated for Cr^{3+} centers in $PbTiO_3$ [7], this multi-constraint strategy significantly reduces ambiguity in defect assignment by eliminating chemically or structurally inconsistent configurations.

The integration of machine learning-accelerated structural optimization, semi-empirical modeling, and charge validation provides a reliable, cost-effective pathway for defect identification. This framework directly correlates local structure, charge distribution, and EPR observables, enhancing the reliability of spectroscopic interpretation. Applications to representative defect centers demonstrate the effectiveness of this approach in distinguishing competing models and providing physically meaningful insights into defect structure–property relationships, offering a generalizable tool for complex materials.

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[7] YB Dinler, M Acikgoz, A quantitatively constrained framework for defect identification in oxides: application to Cr3+ centers in PbTiO3, Phys. Chem. Chem. Phys. 28, 9251 (2026).

EMR studies of Magnetic Defects Generated by Grinding Glass-like Carbons

Maria Augustyniak-Jabłokow [a], Roman Strzelczyk [a], Ryhor Fedaruk [a]

[a] *Institute of Molecular Physics, Polish Academy of Sciences, Smoluchowskiego 17, 60-179 Poznan, Poland*
maria.augustyniak@ifmpan.edu.pl

Keywords: glass-like carbon; magnetic susceptibility, surface effects, exchange interactions, superantiferromagnetism,

EMR studies require appropriate preparation of carbon samples. Powdering electrically conductive materials avoids resonance line asymmetry due to a skin effect. Dilution in a diamagnetic medium allows for the preparation of samples small enough to avoid Rabi splitting effects [1]. The developed surface of powdered samples requires protection from contact with oxygen, hence they should be studied in a vacuum or a protective atmosphere. However, such sample preparation does not always guarantee success. In the case of anthracite, we have previously observed differences between the EMR spectra of diluted powders and small platelets with thicknesses below the skin layer depth [2].

Our study of nonconducting glassy carbon (GLC) obtained from polymerized furfuryl alcohol by pyrolysis at 600 ºC reveals that the number of paramagnetic centers increases with temperature leading to a non-Curie temperature dependence of susceptibility. Additionally, a significant discrepancy between the susceptibility measured by EMR and DC magnetometry is observed. DC magnetometry shows the presence of ferromagnetically ordered phase. However, the EMR study of the large bulk GLC sample reveals only a narrow signal characteristic for the exchange interacting paramagnetic centers. At the same time, in large powdered samples, broad additional signals are clearly visible. This means that conditions for their appearance are created by grinding, which significantly increases the surface area of the GLC. In the temperature range 100-296 K the broad EMR signals have a constant intensity suggesting that they arise from ferromagnetically coupled centers. This hypothesis is supported by observation of a narrow magnetic hysteresis. Such grinding-induced ferromagnetism is observed for nanoparticles of antiferromagnetic materials [3, 4] and interpretated as manifestation of superantiferromagnetism described by Neel [5]. This justifies conclusion that the studied GLC is a diluted antiferromagnet.

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[5] Néel, L. *CR Acad. Sci*, *253*, 203-208 (1961).

New functionalities in multiharmonic analysis

Tomasz Czechowski [a], Mikołaj Baranowski [a,b], Piotr Szczepanik [a], Piotr Jurga [a],
Paweł Malinowski [a]

[a] *Novilet, 1 Romana Maya, Poznań, Poland*
[b] *Faculty of Physics and Astronomy, Adam Mickiewicz University in Poznan, Poland*
t.czechowski@novilet.eu

Multiharmonic analysis has been developed for years [1–5] and enables, among other things, the reconstruction of the unmodulated shape of CW EPR spectra regardless of the modulation amplitude used. Ultimately, the quality of the obtained signals is influenced by experimental parameters, hardware parameters, and the analysis algorithms used. Properly performed multiharmonic analysis requires consideration of a number of factors, in particular: the impact of the detection bandwidth on the recorded harmonics and the passage effect in the recorded data.

The solutions used in the new algorithm allow for the correction of these effects and the acquisition of spectra unaffected by these factors. Firstly, this results in signal reconstruction with the highest possible efficiency, even if the signal's bandwidth was wider than the detection bandwidth. Secondly, it is possible to perform multiharmonic analysis for radicals for which the passage effect known from the rapid scan technique is observed on the harmonics, which is corrected during the analysis. Additionally, the procedures used in the multiharmonic analysis algorithm to optimize the noise parameters of the spectrum provide an above-average increase in sensitivity. The use of multiharmonic analysis results in a multiple increase in the signal-to-noise ratio of the spectra, which, depending on the experimental conditions, can reach up to two orders of magnitude.

It should be emphasized that the development and practical implementation of multiharmonic analysis has been significantly advanced thanks to the work of Novilet, whose technological solutions and innovative algorithms played a key role in refining this technique. Multiharmonic analysis can be performed on Novilet ERI DUO imagers or as an add-on to existing or new Bruker EPR spectrometers.

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Applications of EPR spectroscopy in the analysis of ROS quenchers in Fenton-type reactions

Wiktor Czerwonka[a,b], Kamila Sobańska[a], Piotr Pietrzyk[a]

[a] *Jagiellonian University, Faculty of Chemistry, ul. Gronostajowa 2, 30-387, Krakow, Poland*
[b] *Jagiellonian University, Doctoral School of Exact and Natural Sciences, ul. Prof. St. Łojasiewicza 11, 30-348 Kraków, Poland*
wiktor.czerwonka@doctoral.uj.edu.pl

Keywords: Fenton-like reaction, reactive oxygen species, advanced oxidation processes, spin trapping, spin labelling

The advanced oxidation processes (AOPs) based on hydrogen peroxide offer a versatile approach to eliminating persistent organic contaminants, such as dyes, pesticides and pharmaceuticals, from industrial effluents. The effectiveness of the aforementioned substances is derived from their ability to generate reactive oxygen species (ROS) in a localised manner. This predominantly includes hydroxyl radicals (•OH) and singlet oxygen ($^1O_2$). The presence of ROS initiates an oxidative transformation and, under optimal conditions, the mineralisation of highly resistant molecules. One method for detecting the radicals generated during such reactions is the utilization of EPR spectroscopy, whereby spin trapping, spin probes and direct measurements of surface superoxide species are employed. Another technique involves using scavengers for reactive oxygen species during the degradation of model pollutants. As scavengers react more rapidly with ROS, they slow down the pollutant's degradation and reduce its degree of decomposition after a specified time. Furthermore, using selective scavengers enables the contribution of specific ROS to pollutant degradation to be determined. However, it is important to note that certain redox catalysts are not susceptible to scavenging, and in some cases, scavengers can actually accelerate the reaction. In this study, a series of synthesised using solvothermal and precipitation routes heterogeneous, copper based, Fenton-like catalysts were examined in terms of the reactive oxygen species they generate and their interaction with selected quenchers. This examination was conducted using the EPR spectroscopy techniques mentioned earlier. The overarching objective of the present research endeavour is to assess the evolution of ROS speciation in relation to catalyst composition and surface state. Such studies are anticipated to enhance the precision of structure-activity-selectivity relationships, thereby furnishing a more robust foundation for the optimisation of catalysts under authentic water treatment conditions.

Acknowledgement: This work was financially supported by the National Science Center, Poland (NCN), grant OPUS27 2024/53/B/ST4/03929.

Rabi Oscillations of Paramagnetic Centers with Short Relaxation Times: Peculiarities of Observation and Simulation

Ryhor Fedaruk [a], Antonio Barbon [b], Grigory A. Rusetsky [c], Sveva Linarello [b], Roman Strzelczyk [a]

[a] Institute of Molecular Physics, Polish Academy of Sciences, Smoluchowski Str. 17, 60-179 Poznan, Poland
[b] Department of Chemical Sciences, University of Padova, via Marzolo 1, 35131 Padova, Italy
[c] Scientific-Practical Material Research Centre, Belarus National Academy of Sciences, 19 P. Brovka Str., Minsk 220072, Belarus
ryhor.fedaruk@ifmpan.edu.pl

Keywords: EPR, Rabi oscillations, short spin relaxation times, shaped pulse

In pulsed EPR, Rabi oscillations (transient nutations) are used to determine electron spin multiplicities, discriminate allowed and forbidden transitions, separate overlapping EPR spectra, and study solid-state spin qubits which have a variety of applications in quantum information technologies. They are successfully applied when the Rabi frequency significantly exceeds the spin relaxation rates. However, the short transverse relaxation time, being comparable to or even shorter than the dead time of EPR spectrometers (a typical value about 80 ns at X-band), makes it difficult to observe and describe Rabi oscillations.

In the present report, peculiarities of observation and simulation of Rabi oscillations of paramagnetic centers with short relaxation times are considered. We demonstrate that in this case the frequency of Rabi oscillations depends not only on the intensity of the microwave pulse, but also on its shape and relaxation rates. At short relaxation times, Rabi oscillations cannot be detected directly during the exciting MW pulse or after the pulse by measuring a primary or rotary spin echo, and only the FID detection can potentially be used. Two techniques suitable for this purpose are considered in which Rabi oscillations are detected by monitoring the FID amplitude as a function of pulse duration or microwave field amplitude. We describe the FID-detected Rabi oscillations analytically or numerically for rectangular or shaped pulses, respectively. The description is confirmed by EPR experiments using DPPH ($T_2 = T_1 = 89 \pm 7$ ns) as a model sample [1].

The applicability of the proposed measurement protocol with varying the MW amplitude have recently been demonstrated for fast-relaxing spins in glass-like carbon [2] where the relaxation times ($T_2 = T_1 = 35$ ns) were about three times shorter than in DPPH.

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Electron Paramagnetic Resonance of Transition-Metal Activators in Luminescent Oxides – Case Study: Mn^{4+} Ions

Yatramohan Jana [a], Ireneusz Stefaniuk [b], Czesław Rudowicz [c]

[a] *Department of Physics, University of Kalyani, Kalyani -741235, Nadia, W.B., India*
[b] *Institute of Materials Engineering, University of Rzeszów, Pigonia 1, Rzeszów 35-939, Poland*
[c] *Faculty of Chemistry, Adam Mickiewicz University, Poznań 61-614, Poland*
ymjana@klyuniv.ac.in

Key words: EPR; Transition-metal ions ($3d^N$, $4f^N$); Crystal (ligand)-field; Spin-Hamiltonian parameters; Mn^{4+}-activated luminescent oxides

Transition-metal ions (TMI: $3d^N$, $4f^N$) are widely used as activators in luminescent materials, as their optical properties are strongly governed by oxidation state, crystal-field (CF) strength, and site symmetry. Among these, Mn^{4+}-activated oxides have attracted significant attention as efficient red-emitting phosphors for optoelectronic applications. Reliable identification of valence state and coordination environment is, therefore, essential for designing and tailoring the physical properties of TMI-activated oxide phosphors. EPR provides a powerful *microscopic probe*, directly revealing the spin states, zero-field splitting (ZFS), and CF effects [1]. EPR is also an effective tool for identifying radical species and assessing pollutant levels, including environmentally persistent and biogenic free radicals, underscoring its versatility across solid-state, environmental, and biological systems.

This plenary lecture overviews EPR investigations on TMI activators in luminescent oxides, with emphasis on Mn^{4+} ($3d^3$) centers in octahedral coordination. We show how the CF energy levels, and thus the spin-Hamiltonian parameters (g-factors and ZFS parameters) can be reliably modelled using the exchange charge model and/or superposition model to enable correlation with lattice distortions and site symmetry [1]. The role of orbit-lattice interactions and strain-induced distortions in modifying CF energy levels and ZFS [1] will be also addressed.

As case study, the results for Mn-doped oxides, e.g., pyrochlore Y_2GaSbO_7:Mn^{4+} [2] and double perovskite $BaSrYTaO_6$:Mn^{4+}, will be presented. Temperature-dependence of EPR spectra, which provides evidence for Mn^{4+} centers and reveals characteristic spectral features, is also discussed. These results are correlated with photoluminescence to establish structure-property relationships. Overall, the lecture will demonstrate the effectiveness of EPR in elucidating the CF levels and spin levels of TMI activators, with Mn^{4+} systems providing representative examples.

[1] (a) Biswas *et al.*, Effects of distortions in ion-host systems on optical spectra, crystal-field and spin-Hamiltonian parameters of Cr^{3+} ions doped pyrochlores $Y_2Ti_2O_7$ and $Y_2Sn_2O_7$: exchange charge model and superposition model calculations, PCCP **25** (2023) 5082; (b) Biswas *et al.*, Orbit-lattice interaction, induced structural distortions and lattice strain affecting energy levels of Ni^{2+} ions doped pyrochlores: $Y_2Ti_2O_7$ and $Gd_2Ti_2O_7$, Comput. Mater. Sci. **240** (2024) 113016.

[2] Y.M. Jana *et al.*, Tuning structural, spectroscopic and electronic properties of Mn^{4+} doped Y_2GaSbO_7 phosphor for optoelectronics and phototherapy applications, J. Alloy. Compd. **1037** (2025) 182169.

Hydroxyl Radical Scavenging by Metal Oxide Nanoparticle Catalysts for Enhanced Stability of Alkaline Fuel Cells

Krzysztof Kruczała [a], Bartłomiej Grzywa [a], Szymon Wierzbicki [a,b]

[a] *Faculty of Chemistry, Jagiellonian University, Gronostajowa 2, 30-387, Kraków, Poland*
[b] *Doctoral School of Exact and Natural Sciences, Jagiellonian University, Gronostajowa 2, 30-387, Kraków, Poland*
kruczala@chemia.uj.edu.pl

Keywords: fuel cells, radical scavengers, oxide nanoparticles, competitive kinetics

Electrochemical energy storage and conversion technologies, including flow batteries, electrolyzers, and fuel cells (FCs), are central to the renewable energy supply chain. While proton-exchange membrane fuel cells are technologically mature, their reliance on scarce noble metals limits large-scale deployment. Anion-exchange membrane fuel cells (AEMFCs) offer a promising alternative because non-PGM catalysts and less expensive hydrocarbon membranes can be used under alkaline conditions. However, AEMFC durability is still limited by degradation of hydroxide-conducting ionomers, which decreases membrane-electrode assembly performance and promotes catalyst agglomeration [1]. Using operando EPR, we previously demonstrated radical formation during AEMFC operation on both PGM and non-PGM catalysts, including Fe-N-MWCNT systems [2,3]. EPR spectra of DMPO-OH adducts recorded from a Pt/C-coated cathode placed directly in the spectrometer cavity confirmed hydroxyl radical generation during FC operation. In this work the radical-scavenging properties of commercially available TiO_2, synthesized Ru-doped TiO_2 (RTO), and CeO_2 were evaluated under alkaline conditions.

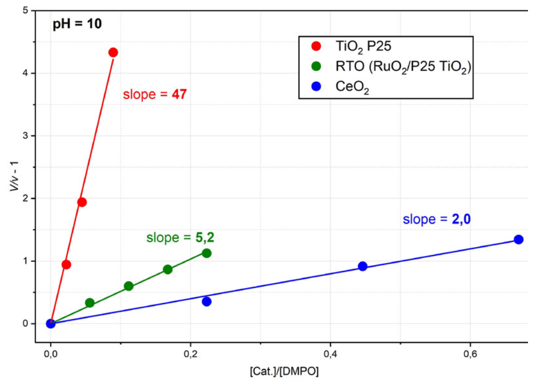

Fig. 1. CK plots for ORR catalysts supports: XC-72 carbon, TiO_2 and RTO.

A competitive kinetic (CK) approach based on spin-trapping EPR was applied to quantify the hydroxyl-radical scavenging ability of the investigated oxide systems [4]. For a linear CK plot (**Fig. 1**), the slope corresponds to k_C/k_{DMPO} and provides a quantitative measure of hydroxyl-radical quenching efficiency: higher slope indicates more effective radical scavenging.

Acknowledgements: This work was supported by the NCN under Grant No. 2024/53/B/ST4/01150.

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Two-dimensional ferromagnetism in Cr_3Te_4

Marian Kuźma

University of Rzeszow, Institute of Physics, Pigonia 1, 35-959 Rzeszów, Poland
mkuzma@ur.edu.pl

Keywords: two-dimensional ferromagnetism, EPR, Cr_3Te_4.

The 3d metal chalcogenides (MC) is known class of materials in which the idea of 2D magnetism can be realized. The crystal structure of bulk crystals of such materials is layered, in which the atoms within the layer are bound by strong covalent bonds, while weak van der Waals bonds act between the layers.

Bulk crystals can be used to obtain layers (monolayers) containing several or more atomic layers, either by thinning a bulk sample into a thick layer on a substrate or by exfoliation. Monolayers are two-dimensional objects and exhibit physical properties distinct from bulk crystals. However, the use of monolayers in spintronics is limited because, according to the Mermin-Wagner theory, long-range magnetic order (ferromagnetism, antiferromagnetism) does not exist in a two-dimensional system. Combining ferromagnetic properties (if such existed in 2D materials) with their unique optical or electrical properties will open up new applications in magnetooptical or magnetoelectric devices.

The first 2D materials in which long-range magnetic order was observed were CrI_3 [1] and $Cr_2Ge_2Te_6$ [2]. It turned out that such long-range order is possible due to the high magnetic anisotropy in these materials. Recently, extensive studies on two-dimensional magnetism have been conducted for a group of transition metal sulfides materials. Some of these materials have high Curie temperatures, approaching room temperature. In this paper, we focus on Cr_3Te_4, whose Curie temperature in bulk crystals is 306-314 K. We demonstrate that the source of magnetic anisotropy is double superexchange as a result of the structure of Cr_3Te_4 crystals. We explain the role of the magnon spectrum in the emergence of long-range order in monolayers.

We have measured EPR spectra for polycrystalline Cr_3Te_4. The temperature dependence of the spectra have been analyzed in the frame of magnon approach to the dynamic spin susceptibility depending on the wave vector and the frequency [3]. This model enables to estimate the ratio of J_{perp}/J_{par} of quasi-two dimensional Cr_3Te_4.

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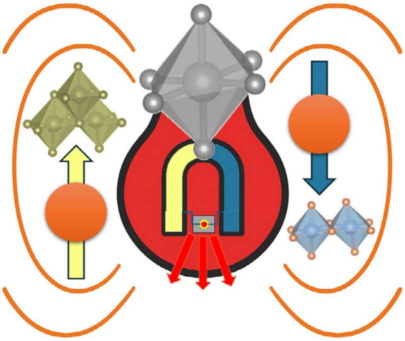
Decoding Broadband NIR Luminescence through EPR in Cr^{3+}-Activated Mixed Spinels

Grzegorz Leniec [a,b], Ewa Mijowska [a,b], Sebastian Mahlik [c], Ru-Shi Liu [d]

[a] Department of Nanomaterials Physicochemistry, Faculty of Chemical Technology and Engineering, West Pomeranian University of Technology in Szczecin, Piastów Ave. 45, 70-311 Szczecin, Poland
[b] West Pomeranian University of Technology in Szczecin, Faculty of Chemical Technology and Engineering, Center for Advanced Materials and Manufacturing Process Engineering MATPRO, al. Piastów 42, 71-065 Szczecin, Poland
[c] Institute of Experimental Physics, Faculty of Mathematics, Physics, and Informatics, University of Gdansk, Wita Stwosza 57, 80-308 Gdańsk, Poland
[d] Department of Chemistry, National Taiwan University, Taipei 106, Taiwan
gleniec@zut.edu.pl

Keywords: luminescence, spinel, chromium, single Cr^{3+}, Cr^{3+} pairs, Cr^{3+} clusters



The spectroscopic properties of Cr^{3+}-activated spinels are governed by variations in the local crystal-field environment, cation disorder, and Cr–Cr magnetic interactions, all of which directly influence near-infrared (NIR) emission characteristics. In this presentation, electron paramagnetic resonance (EPR) spectroscopy was combined with photoluminescence spectroscopy to establish correlations between paramagnetic Cr^{3+} centers and their emission properties in the mixed spinel system $Mg(Ga,Al)_2O_4{:}0.06Cr^{3+}$.

Optical spectroscopy reveals systematic modifications of the crystal-field strength through the energetic evolution of the $^4T_2$ and ^2E states, while EPR provides direct insight into local symmetry, exchange interactions, and the distribution of isolated Cr^{3+} ions, exchange-coupled Cr–Cr pairs, and cluster-like centers. Particular attention is devoted to the evolution of EPR line shape, linewidth broadening, and effective g-factor variations as a function of the Ga/Al ratio, reflecting changes in short-range structural disorder and magnetic coupling pathways.

The combined spectroscopic analysis demonstrates that the broadband NIR emission originates from a heterogeneous distribution of Cr^{3+} environments rather than from a single crystallographic site. The relative contributions of isolated ions and magnetically interacting centers are shown to strongly affect emission bandwidth and spectral position. These results provide a direct spectroscopic link between local paramagnetic structure and luminescence properties in Cr^{3+}-activated spinels.

The presented EPR–luminescence correlation offers a framework for the targeted engineering of broadband NIR phosphors based on controlled crystal-field tuning and defect-assisted formation of interacting Cr^{3+} centers.

EPR Spectroscopy of Radiation-Induced Centers in Borate Crystals and Glasses (Review)

Bohdan Padlyak

Ivan Franko National University of Lviv, O.G. Vlokh Institute of Physical Optics, Dragomanov Str. 23, 79-005 Lviv, Ukraine
bohdan@mail.lviv.ua

Keywords: borate compounds, irradiation, EPR, radiation-induced centers, superhyperfine structure.

In this review our and other articles [1–5] devoted to EPR studies of the radiation-induced centers in crystalline and glassy borate compounds are considered and discussed. In particular, the X-band (ν ≅ 9.4 GHz) EPR spectra of borate glasses with $Li_2B_4O_7$, $LiKB_4O_7$, LiB_3O_5, $LiCsB_6O_{10}$, CaB_4O_7, SrB_4O_7, and SrB_6O_{10} chemical compositions, which were irradiated by high dose of the γ - ray (10^7 Gy) and X - ray ($1 \div 2 \cdot 10^4$ R) at room temperature are detailed analyzed and interpreted.

The X - and γ - irradiation at RT of the investigated borate glasses with different chemical compositions leads to generate 3 types of stable paramagnetic centers, which have been identified by EPR spectroscopy and denoted by us: RC 1, RC 2, and RC 3. The efficiency of generation and type of the radiation-induced paramagnetic centers weakly depends on the basic borate glass composition (i.e., ratio of the network former to the modifiers) and practically is independent of the kind of ionizing radiation (X or γ) as well as presence of the Fe^{3+} non-controlled impurity ions in the glass network. EPR spectra of most intense RC 1 centres are characterized by hole-like g - factor ($g \cong 2.014$) and can be described in the framework of model of the ensemble of O^- hole centers (or BOHC), located in different sites of non-bridging oxygen of borate glass network. The 4-component EPR spectrum of the O^- centers are related to the superhyperfine (SHF) structure ($a \cong 1.3$ mT), caused by interaction of the unpaired electron spin with one nearest nucleus of the ^{11}B magnetic isotope (nuclear spin $I = 3/2$, natural abundance – 80.1 %). The weak EPR signal with 7-component SHF structure belong to the O^- centers, localized near one nucleus of the ^{10}B isotopes (nuclear spin $I = 3$, natural abundance – 19.9 %). Observed in the X - and γ - irradiated borate glasses unstructured broad EPR signal of the RC 2 centers can be attributed to the ensemble of O^- hole centers ($g \approx 2.041$), located in the positions of bridging oxygens far from magnetic isotopes of glass network. The RC 3 signal ($g \cong 1.961$), observed in the $Li_2B_4O_7$ glass can be attributed to centers of the electron type and their nature needs additional more detailed study.

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Temperature-Dependent EPR Study of Powder Coatings

Piotr Pisiak [a], Bogumił Cieniek [a], Ireneusz Stefaniuk [a]

[a] University of Rzeszow, Institute of Materials Engineering, Pigonia 1, 35-959 Rzeszow, Poland
piotrp@dokt.ur.edu.pl

Keywords: powder coatings, EPR spectroscopy, laser irradiation, polyester resins, paramagnetic centers

Powder coatings are widely used in industry because of their high mechanical strength and chemical resistance. In this study, commercially available powder coatings were examined using electron paramagnetic resonance (EPR) spectroscopy to analyze structural defects and paramagnetic centers in polymeric coating materials. Measurements were performed in the temperature range of 300–500 K. The EPR spectra revealed broad resonance lines characteristic of complex paramagnetic systems. The observed changes in all line parameters indicate alterations in the local environment of paramagnetic centers and defect-related structures in polyester powder coatings.

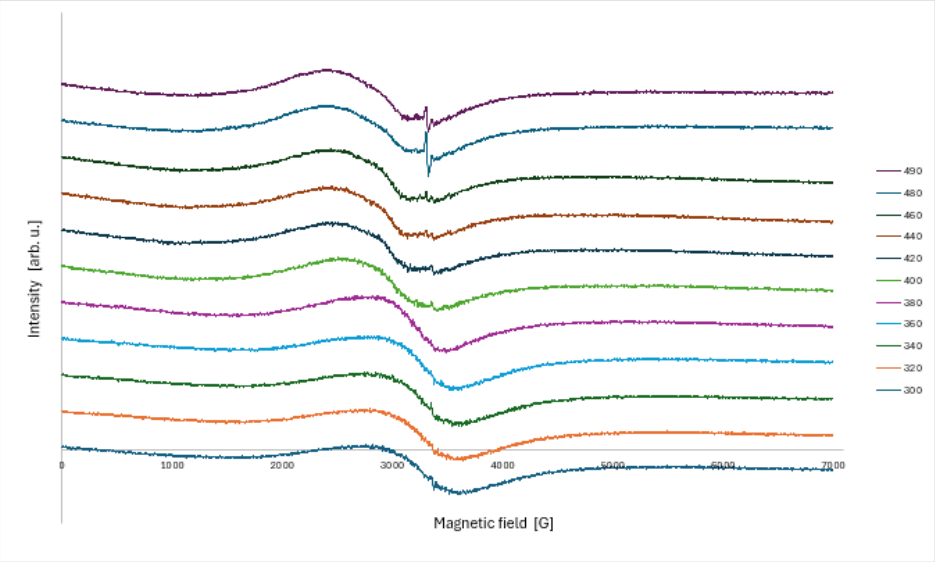

Figure. 1. Temperature dependence of the EPR spectra of powder paint

EPR Study of APTES/TiO_2 Nanomaterials with Temperature-Dependent Properties

Danuta Piwowarska [a], Niko Guskos [a], Czesław Rudowicz [b], Ireneusz Stefaniuk [c],
Bogumił Cieniek [c], Agnieszka Wanag [d], Ewelina Kusiak-Nejman [d],
Antoni W. Morawski [d]

[a] *West Pomeranian University of Technology in Szczecin, Faculty of Mechanical Engineering and Mechatronics, al. Piastów 19, 70-310 Szczecin, Poland*
[b] *Adam Mickiewicz University, Faculty of Chemistry, 61-614 Poznań, Poland*
[c] *University of Rzeszów, Institute of Materials Engineering, Pigonia 1, 35-959 Rzeszów, Poland*
[d] *West Pomeranian University of Technology in Szczecin, Department of Inorganic Chemical Technology and Environment Engineering, Pułaskiego 10, 70-322 Szczecin, Poland*
danuta.piwowarska@zut.edu.pl

Keywords: EMR/EPR; Titanium dioxide(TiO_2); 3-Aminopropyltriethoxysilane (APTES), oxygen vacancy; Spin Hamiltonian.

The paramagnetic centers created in titanium dioxide modified with 3-aminopropyltriethoxysilane (APTES) powders were probed by the electron paramagnetic resonance (EPR) spectroscopy at liquid nitrogen temperature. The nanomaterials based on TiO_2 modified with APTES: TiO_2-4h-180^{0}C-500mM-800°C (sample 1), TiO_2-4h-180^{0}C-500mM-900°C (sample 2) and TiO_2-4h-180^{0}C-500mM-1000°C (sample 3) were obtained by solvothermal processes, thermal modification in the argon atmosphere and calcination at 800°C, 900°C and 1000°C.

The EPR spectra recorded in temperature range 80 - 300 K for the samples (1) – (3) reveal the presence of an electron trapped on an oxygen vacancy (V0) with of the sharp signal (L1) centered between geff = 2.0025(7) and geff = 2.0028(9). Additionally, the EPR broad signal (L2), observed only at temperatures below 135 K for samples 2 and 3, indicates the existence of some Ti^{3+} ions located at low coordination sites. The signal (L2) was centered between g_{eff} = 1.9565(8) and g_{eff} = 1.9750(4).

The temperature dependence of EPR integrated intensities has shown the presence of different relaxation processes at various temperature ranges. These differences may arise from varying concentrations of conduction electrons in the samples. The two types of EPR signals observed in our study may be attributed to existence of distinct paramagnetic centers. Modifying titania with APTES has been found to lead to enhanced photocatalytic properties compared with unmodified TiO_2 calcined at the same temperatures.

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Study of electron magnetic resonance in heavily Cr-implanted CdTe single crystals with dopant-related secondary phases

Volodymyr Popovych [a,b], Andrii Popovych [a], Bogumil Cieniek [c], Piotr Dłużewski [d], Antoni Żywczak [e], Ihor Stolyarchuk [a], Makoto Shiojiri [f], Marian Kuźma [g]

[a] *Department of Technological and Professional Education, Drohobych State Pedagogical University I.Franko, I.Franko 24, 82100, Drohobych, Ukraine*
[b] *Department of Computational Mathematics and Programming, Lviv Polytechnic National University, Stepan Bandera Str. 12, 79000 Lviv, Ukraine*
[c] *University of Rzeszow, Institute of Materials Engineering, Pigonia 1, 35-959 Rzeszow, Poland*
d Institute of Physics, Polish Academy of Sciences, Aleja Lotników 32/46, Warsaw, 02-668, Poland
[e] *AGH University of Science and Technology, Academic Centre for Materials and Nanotechnology, Kawiory 30, 30-055 Kraków, Poland*
[f] *Kyoto Institute of Technology, Matsugasaki, Sakyo-ku, 606-8585 Kyoto, Japan*
[g] *University of Rzeszow, Institute of Physics, Pigonia 1, 35-959 Rzeszow, Poland*
vpopovych@dspu.edu.ua

Key words: CdTe, Cr^+ implantation, magnetic resonance, magnetization, nanoprecipitates.

The {110}-oriented samples were prepared from vapor-grown CdTe single crystals, and then implanted with 500 keV Cr^+ ions at fluences up to $5\cdot10^{17}$ cm^{-2} to overcome the low equilibrium solubility of this element in the CdTe lattice. Using HAADF-STEM and EDXS, it was revealed that implantation induces phase separation and the formation of dopant-related particles with sizes of 10−40 nm at depths up to 500 nm from the irradiated surfaces. These were identified as precipitates of the monoclinic Cr_3Te_4 with the $(3\bar{1}\bar{3})_{Cr_3Te_4}\|(20\bar{2})_{CdTe}$ and $[101]_{Cr_3Te_4}\|[111]_{CdTe}$ orientation relationships with respect to the host matrix, which are known to be ferromagnetic at RT.

Magnetization measurements revealed ferromagnetic ordering in the implanted samples at LNT and RT, with low-coercivity hysteresis loops characteristic of soft magnetic materials. Their magnetic resonance properties were investigated using a 9.43 GHz X-band Bruker FT-EPR spectrometer over the 100–300 K range. The samples exhibit broad, asymmetric resonance lines, which at RT can be fitted with two broad Lorentzian components, indicating magnetically non-equivalent resonance contributions associated with different local anisotropy conditions within the ensemble of ferromagnetic nanoprecipitates. A weak contribution from the surrounding $Cd_{1-x}Cr_xTe$ matrix cannot be completely excluded.

Upon cooling, the resonance line progressively broadens, becomes strongly distorted, and its peak intensity decreases substantially. The observed temperature evolution may arise from strong inhomogeneous broadening of the FMR absorption due to enhanced magnetic anisotropy, stronger internal magnetic fields, and increasing interparticle dipolar interactions. The shift of the resonance toward lower magnetic fields with decreasing temperature is attributed to an increase in the effective internal magnetic field associated with spontaneous magnetization. The results are consistent with magnetic blocking in an ensemble of ferromagnetic Cr_3Te_4 nanoprecipitates upon cooling below approximately 220 K.

Importance of Tesseral and Spherical Tensor Operators for Describing Low-Symmetry Aspects in EMR and Optical Spectroscopy

Czesław Rudowicz [a], Sushil K. Misra [b], Ireneusz Stefaniuk [c], Muhammed Açıkgöz [d]

[a] *Faculty of Chemistry, Adam Mickiewicz University, Poznań 61-614, Poland*
[b] *Physics Department, Concordia University, Montreal, QC H4B 1R6, Canada*
[c] *University of Rzeszow, Institute of Materials Engineering, Pigonia 1, 35-959 Rzeszów, Poland*
[d] *Department of Science, State University of New York, Maritime College, New York 10465, USA*
czeslaw.rudowicz@amu.edu.pl

Keywords: EMR/EPR; Optical spectroscopy; Spin Hamiltonian (SH); Crystal (ligand)-field Hamiltonian; Low-Symmetry Aspects; Transition metal ions ($3d^N$, $4f^N$).

Electron magnetic resonance (EMR) and optical spectroscopy enable characterization of transition metal 3d/4f ions in coordination compounds, which often exhibit low (monoclinic or triclinic) symmetry sites. Low symmetry aspects (LSAs) are largely unexplored as yet due to lack of adequate knowledge. Thus they are often neglected and orthorhombic or higher symmetry approximations are employed instead. To alleviate these problems, the key notions are elucidated to provide valuable insights in EMR, optical spectroscopies, magnetism and related areas [1].

Categorization of high and low site symmetry cases is provided based on point symmetry groups (PSGs) and the unique character of orthorhombic site symmetry is exposed [1]. The LSAs, including the low symmetry effects (LSEs) observable in EPR spectra of 3d/4f ions with spin S > ½, cannot be described using the *conventional* 2nd-rank zero-field splitting (ZFS): $H_{ZFS} = \boldsymbol{S.D.S}$. The tensor operators of the rank k = 2, 4, 6 play crucial role in EMR and optical spectroscopy in describing LSAs and LSEs. The tesseral tensor operators (**TTO**) - Stevens operators (SO): extended SO (ESO) and generalized (GESO), and the spherical tensor operators (**STO**), as well as respective ZFS parameters (ZFSPs) are overviewed to clarify their mutual relationships [2].

Fundamentals of the spin Hamiltonian and the crystal field (CF) Hamiltonian are briefly presented [1]. This includes: (i) role of PSGs and site symmetry in spectroscopy, (ii) symmetry-adapted axis systems and crystallographic axis systems, (iii) crystallographically and magnetically inequivalent sites in crystals, (iv) triclinic and symmetry-specific forms of spin Hamiltonians, (v) distinctions between H_{ZFS} and H_{CF}, (vi) laboratory and magnetic axis systems.

The intricate problems encountered in the fitted and modelled ZFSP sets for Gd^{3+} ions at trigonal and triclinic sites in dinuclear complexes [3] are discussed. Our study [3] reveals serious inadequacy of the packages SHAPE as well as DFT-based MOLCAS for ZFSP modelling.

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EPR insight into the role of H_2O_2-derived ROS in the degradation of model water pollutants

Kamila Sobańska[a], Łukasz Wolski[b], Piotr Pietrzyk[a]

[a] *Jagiellonian University, Faculty of Chemistry, Gronostajowa 2, 30-387 Kraków, Poland*
[b] *Adam Mickiewicz University, Faculty of Chemistry, Uniwersytetu Poznańskiego 8, 61-614 Poznań, Poland*
kamila.sobanska@uj.edu.pl

Keywords: reactive oxygen species, hydrogen peroxide, spin trapping, advanced oxidation processes

Increasing environmental contamination with persistent organic pollutants, including dyes, pharmaceuticals, and other emerging contaminants, has become a major environmental concern due to their toxicity, chemical stability, and resistance to conventional wastewater treatment methods. In this context, advanced oxidation processes (AOPs), particularly Fenton and Fenton-like reactions together with their modifications, have attracted considerable attention as effective methods for the degradation and mineralization of recalcitrant organic contaminants. These processes are based on the generation of reactive oxygen species (ROS), such as hydroxyl radicals ($^{\bullet}OH$), superoxide radical anions ($O_2^{\bullet-}$), and singlet oxygen ($^1O_2$), which exhibit exceptionally high oxidative activity toward a broad range of organic pollutants. ROS are typically generated through reactions involving hydrogen peroxide, enabling efficient oxidation without the formation of secondary toxic by-products. Owing to their high efficiency, AOPs are increasingly considered a valuable complement or alternative to conventional biological, mechanical, and chemically assisted purification methods, particularly as a final polishing step for the removal of low concentrations of persistent contaminants from aqueous systems. The effectiveness of these processes strongly depends on the properties of the applied catalyst, as its composition and structure determine the generation efficiency of highly reactive oxidizing species.

In this work, reactive oxygen species were identified, and the influence of catalyst composition (type of transition metal and presence of dopants) on their formation was investigated. The generation of reactive oxygen species was confirmed by EPR spectroscopy using spin trapping with DMPO and oxidation of TEMP, enabling the identification of hydroxyl radicals ($^{\bullet}OH$) and singlet oxygen, respectively. In addition, the catalytic activity was evaluated in the degradation of organic dyes (methylene blue and rhodamine B) as well as the antibiotic ciprofloxacin. The obtained results demonstrated a synergy between the adsorption of pollutant molecules on the catalyst surface and the catalytic activity in generating reactive oxygen species, including both hydroxyl radicals and singlet oxygen, as well as their effectiveness in the degradation of contaminants.

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Binding and Activation of Selected Small Molecules on Metallozeolites – Spectroscopic and DFT Insights

Zbigniew Sojka

Jagiellonian University, Faculty of Chemistry, ul. Gronostajowa 2, 30-387 Krakow, Poland
sojka@chemia.uj.edu.pl

Keywords: metallozeolites, small molecules, EPR, DFT catalysis, adsorption, activation

The chemistry of metallozeolites exchanged with 3d transition metals has attracted wide attention over the years due to their well-defined framework structures, redox flexibility, and remarkable adsorption and catalytic properties, as well as their vital relevance for chemical technology. The binding and activation of small reactant molecules are essential components of comprehensive experimental and theoretical investigations into the mechanistic complexity of the involved intrazeolite reactions and the associated processes. It is governed by the intricate mechanistic interplay of intrazeolite reactions, which are influenced by the flexible valence, spin, and coordination states of the encapsulated metal ions and their associated metal-oxo entities. The nature of active sites, confinement effects, and the complex activation mechanisms of reactant molecules, which act as both innocent and non-innocent ligands, are discussed at the orbital level. This contribution addresses the following issues: speciation of intrazeolite transition-metal ions, their structural dynamics, and reactivity toward catalytically relevant small molecules, such as CO, N_2, O_2, NO, N_2O, and NH_3. The attention is placed on ligand coordination, redox activation, and the role of electronic and spin states in dictating the catalytic behavior. The discussion integrates insights from site-selective spectroscopies and computational methods to elucidate the structure, metal-ligand interactions, and activation pathways. Particular emphasis is placed on computational spectroscopy applications for molecular interpretation of the spectroscopic EPR parameters of the produced adducts, and their structure sensitivity.

EPR studies of environmentally persistent free radicals and metal ions in various fractions of airborne dust

Ireneusz Stefaniuk [a], Bogumił Cieniek [a], Dariusz Płoch [a], Julia Brewka [b], Katarzyna Kluska [b], Idalia Kasprzyk [b]

[a] *University of Rzeszow, Institute of Materials Engineering, Pigonia 1, 35-959 Rzeszów, Poland*
[b] *University of Rzeszów, Faculty of Biotechnology, Pigonia 1, 35-959 Rzeszów, Poland*
istefaniuk@ur.edu.pl

Keywords: free radicals; EPR; particulate matter; air pollution

The purpose of this study was to analyze airborne particulate matter during the heating season (February and March) and during the off-season (September) over a 2-year period. It also included the Saharan dust inflow reaching southern Poland in the spring of 2025, and was determined to assess its impact on the chemical composition and oxidation potential of airborne particulate matter. Using the ultrasensitive Dekati instrument, aerosols were measured in 15 size fractions (6 nm–10 µm), enabling the detection of even the smallest particles – a feature previously undescribed for Saharan dust [1]. Electron paramagnetic resonance spectroscopy was used to quantify and identify radicals associated with various fractions of particulate matter. The analysis revealed a high content of ultrafine particulate matter (<1 µm), which may pose a potential risk to human health. The use of modern measurement equipment allowed the detection of ultrafine fractions and the identification of free radicals associated with Saharan dust, both during the heating season and outside of it, providing new information on airborne particulate matter, its oxidative potential, and its chemical reactivity.

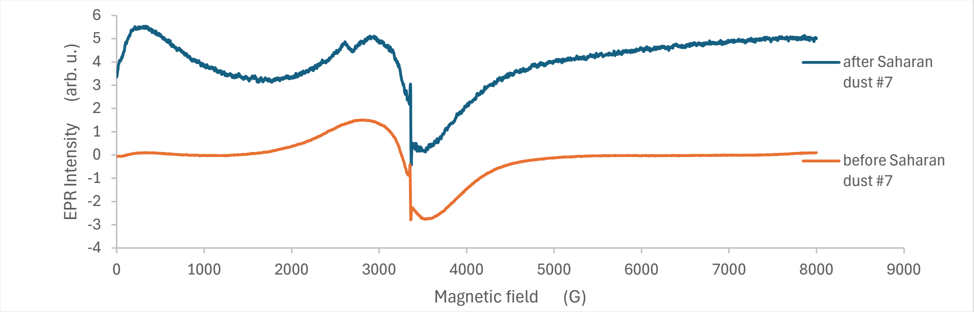

Figure. EPR spectra for filter #7 during the Saharan dust episode (blue line) and during the period without dust influence (orange line).

This research was supported by the Minister of Science of the Republic of Poland under the Programme „Regional initiative of excellence”. Agreement No. RID/SP/0010/2024/1.

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Synthesis and EPR study of the ultrasmall $Zn_{1-x}Mn_xFe_2O_4$ ferrite particles

Anna Tomaszewska [a], Iwona Rogalska [a,b], Bogumił Cieniek [a], Magdalena Kulpa-Greszta [c], Piotr Krzemiński [a], Bartosz Zarychta [d], Ireneusz Stefaniuk [a], Robert Pązik [c]

[a] *University of Rzeszow, Institute of Materials Engineering, Pigonia 1, 35-959 Rzeszów, Poland*

[b] *Institute of Physics, Polish Academy of Sciences, International Research Centre MagTop, Aleja Lotników 32/46, Warsaw, 02-668, Poland*

[c] *University of Rzeszow,Faculty of Biotechnology,, Pigonia 1, Rzeszow 35-959, Poland*

[d] *University of Opole, Faculty of Chemistry, Oleska 48, 45-052 Opole, Poland*

atomaszewska@ur.edu.pl

Keywords: ferrites, EMR, SEM, XRD, magnetic properties.

In this work, we are showing the results of the *X*- and *Q*-band electron magnetic resonance measurements of ultra-small $Zn_{1-x}Mn_xFe_2O_4$ nanoparticles (*c.a.* 8 nm) with a very narrow size distribution. The chosen synthetic route allows for precise structural modifications with a broad concentration range (x – 0, 0.2, 0.5, 0.8, 1). The crystal structure was evaluated by means of the X-ray diffraction technique, while cell parameters were calculated using Rietveld refinement. EMR spectral studies indicated that the prepared nanoparticles were superparamagnetic. The linewidth of EMR signal for any ferrite material generally originates from two sources: (a) magnetic dipole-dipole interactions among particles and (b) interparticle superexchange interactions between magnetic ions through oxygen ions. Observed effects are more complex interactions than in pure zinc and manganese ferrites. As a result of the study, a relationship was observed between the composition of the material and the magnetic properties with striking antiferromagnetism and ferrimagnetism change. Hence, by structural modification of materials, the magnetic character (FM-AFM-FiM) can be controlled.

EMR characterization of high-concentration Co/Cr-doped ZnO films on quartz and sapphire

Ihor Virt [a], Ivan Padalka [a], Bogumił Cieniek [b], Ireneusz Stefaniuk [b]

[a] Department of Physics, Institute of Physics, Mathematics, Economics and Innovative Technologies, Drohobych State Pedagogical University I.Franko, I.Franko 24, 82100, Drohobych, Ukraine
[b] Faculty of Mathematics and Natural Sciences, University of Rzeszów, S. Pigonia 1, 35-959 Rzeszów, Poland
isvirt@email.ua

Keywords: ZnO, Co-doped, Cr-doped, thin films

We have studied magnetic properties of zinc-oxide composite doped with high concentration (up to 20%) of Co and Cr ions. The pulsed laser deposition method was used to obtain samples on quartz glass and sapphire substrates. Samples were annealed at 100–250 ◦C for ZnO on quartz substrate, and 300–700 ◦C on sapphire substrate. EMR measurements were carried out and temperature dependence of the EMR spectra was obtained. The angular dependence in two samples orientation, vertical and horizontal, were also obtained. Analysis of the temperature dependences of the integral intensity of EMR spectra was carried out using the Curie–Weiss law.

With increasing annealing temperature, we observe an increase in paramagnetic properties as a result of weakening of the exchange coupling between Cr and Co ions. Analyzing the behavior of the EMI linewidth for low ion concentration, we argue that the combined effect of exchange and dipole broadening plays an important role in the mechanism of linewidth formation in these materials.

Metal vs Ligand Control of Spin in Cu/Ni Bisamidrazones

Michal Zalibera [a], Iuliana Besleaga [b], Lenka Novotná [a], Ingrid Jelemenská [a], Lukáš Bučinský [a], Peter Rapta [a], Vladimir B. Arion [a,b]

[a] *Institute of Physical Chemistry and Chemical Physics, Faculty of Chemical and Food Technology, Slovak University of Technology in Bratislava, Radlinského 9, SK-812 37 Bratislava, Slovak Republic*
[b] *Institute of Inorganic Chemistry, University of Vienna, Währinger Straße 42, 1090 Vienna, Austria*
michal.zalibera@stuba.sk

Keywords: amidrazone Schiff base, copper, nickel, redox non-innocence, multifrequency EPR, DFT

Pentane-2,4-dione bis(amidrazone) Schiff bases bind first-row metals in a redox-non-innocent tetradentate N_4 pocket. We compare Cu(II/III) and Ni(II/III) amidrazones built on the same scaffold by multifrequency cw-EPR, DFT (B3LYP/def2-TZVP*), electrochemistry, UV-Vis SEC, and Cu K-edge XAS.

The Cu(II) complexes $[Cu(H_2L^R)]^+$ (R = Me, Ph) give axial spectra with $g_\parallel \approx 2.15$, $A_\parallel$ (^{63}Cu) $\approx 215 \times 10^{-4}$ cm^{-1} and ^{14}N superhyperfine - diagnostic of a $d_{x^2-y^2}$ ground state. The formally Cu(III) congeners are EPR silent, but cobaltocene reduction regenerates nearly identical Cu(II) signals. DFT and Cu K-edge XANES corroborate a Cu(II)-$L^{\bullet+}$ rather than d^8 Cu(III) description.

The Ni series behaves oppositely. Ni(II) parents are diamagnetic (low-spin d^8). The formally di-Ni(III) dimer shows near-isotropic $g \approx g_e$ - too small for a Ni-centred radical. Reduced $[Ni(L^{PhO})]^-$ gives a narrow $S = 1/2$ spectrum with a ^{14}N quintet from two equivalent amidrazone N donors (Figure).

The same scaffold thus yields metal-centred spin with Cu and ligand-centred spin with Ni. The d-electron count is decisive: d^9 Cu(II) cannot avoid a hole in $d_{x^2-y^2}$; low-spin d^8 Ni(II) is EPR-silent and leaves the ligand to host the spin. EPR discriminates formal from spectroscopic oxidation state.

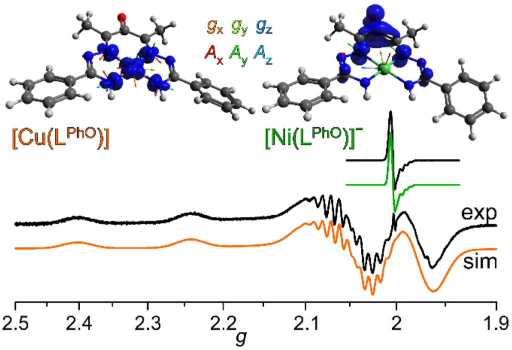

Figure. EPR spectra and DFT predicted spin densities in isoelectronic $[Cu(L^{PhO})]$ and $[Ni(L^{PhO})]^-$

Acknowledgements. Supported by the Slovak Research and Development Agency under contracts APVV-23-0195 and VV-MVP-24-0039, and by VEGA grant 1/0392/24.

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POSTERS

(in alphabetical order)

Tempo-phosphate as an ESR tool to study phosphate transport

Izabela Sadowska-Bartosz [a], Grzegorz Bartosz [a], Bogumił Cieniek [b],
Ireneusz Stefaniuk [b]

[a] *University of Rzeszow, Faculty of Technology and Life Sciences, Institute of Food Technology and Nutrition, Aleksandra Zelwerowicza 4, 35-601 Rzeszów, Poland*
[b] *University of Rzeszów, Institute of Materials Engineering, Pigonia 1, 35-959 Rzeszów, Poland*
gbartosz@ur.edu.pl

Keywords: TEMPO-phosphate; erythrocyte; transport; Band 3 protein

TEMPO-phosphate has been introduced as a phosphate analogue to study phosphate transport in erythrocytes. The nitroxide is reduced intracellularly upon entering the cells, the membrane transport being the rate-limiting step of the loss of the EPR signal. The use of TEMPO-phosphate is convenient and avoids the hazard of radioactivity. We studied the inhibition of TEMPO-phosphate transport to human erythrocytes by various compounds. DIDS and SITS, inhibitors of Band 3, inhibited the TEMPO-phosphate transport. 1-cyano-4-hydroxycinnamic acid, an inhibitor of monocarboxylate transporters, did not affect the permeation of TEMPO-phosphate. The transport of TEMPO-phosphate was inhibited by various polyphenols, especially curcumin, naringin, quercetin, and curcumin.

Compound (100 μM)	**Relative transport rate** [%]
None (control)	100
DIDS	11.4 ± 4.8***
SITS	14.0 ± 7.5**
1-Cyano-4-hydroxycinnamic acid	100.5 ± 3.2
1-Hydroxycinnamic acid	101.1 ± 2.8
Ferulic acid	104.0 ± 5.1
Daidzein	99.5 ± 4.7
Genkwanin	96.8 ± 3.8
Genistein	87.4 ± 5.3*
Kaempferol	87.3 ± 1.9**
Luteolin	76.8 ± 6.2*
Quercetin	74.5 ± 7.1*
Naringin	72.1 ± 6.4**
Curcumin	71.2 ± 5.9**

Application of EPR Spectroscopy as a Tool for Characterizing Copper Biosorption by *Spirulina platensis* and *Chlorella vulgaris*

Bogumił Cieniek[a], Eleonora Sočo[b], Andżelika Domoń[c], Ireneusz Stefaniuk[a]

[a] *University of Rzeszow, Institute of Materials Engineering, Pigonia 1, 35-959 Rzeszow, Poland*
[b] *Rzeszow University of Technology, Department of Inorganic and Analytical Chemistry, 6 Powstańców Warszawy Av., 35-029 Rzeszow, Poland*
[c] *Rzeszow University of Technology, Department of Water Purification and Protection, Faculty of Civil, Environmental Engineering and Architecture, 12 Powstańców Warszawy Av., 35-029 Rzeszow, Poland*
bcieniek@ur.edu.pl

Keywords: EPR spectroscopy; biosorption; copper ions; *Spirulina platensis*; *Chlorella vulgaris*

The growing pollution of aquatic environments with heavy metals calls for increased efforts to identify effective and sustainable biosorbents. Among naturally occurring biomaterials, microalgae such as *Spirulina platensis* and *Chlorella vulgaris* exhibit significant metal ion adsorption capacity due to functional groups in their cellular structure. In this study, electron paramagnetic resonance (EPR) spectroscopy was used to investigate the structural and paramagnetic changes that occur in the *Spirulina platensis* and *Chlorella vulgaris* biomass before and after the adsorption of copper ions from aqueous solutions. The recorded EPR spectra revealed distinct changes in signal intensity, line width, and g-value following the adsorption process, confirming the effective adsorption of copper ions by both biomaterials.

The results obtained show that EPR spectroscopy is a valuable tool for monitoring and characterizing biosorption processes.

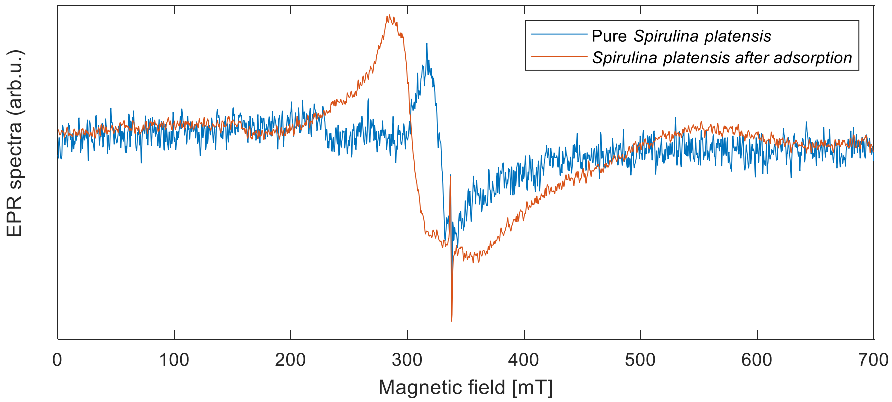

Figure 1. EPR spectra of *Spirulina platensis* before and after copper(II) ions biosorption.

I.I. Rabi was born in Podkarpacie, Poland. Fundamentals of qubits and transient EPR

Mateusz Drąg [a], Tadeusz Jasiński [a], Marian Kuźma [b]

[a] *Department of Physics and Medical Engineering, Faculty of Mathematics and Applied Physics, Rzeszow University of Technology, Powstańców Warszawy str. 6, 35-029 Rzeszów, Poland*
[b] *University of Rzeszow, Institute of Materials Engineering, Pigonia 1, 35-959 Rzeszów, Poland*
m.drag@prz.edu.pl

Keywords: two-level system, Rabi oscilations, qubits

In this report, we recount the life and scientific work of physicist Isydor Isaac Rabi. Isydor Izaak Rabi was born on July 29, 1998, in Rymanów in Podkarpacie in Poland. As a child, he emigrated to America with his parents before World War I. After graduating with a degree in chemical engineering from Cornell University, he quickly earned a doctorate in physics and worked at renowned universities. His work in atomic and nuclear physics pioneered new research and application directions in physics. In his widely known, historic work from 1937 he derived a formula for the probability of transition between Zeeman levels of a particle in a constant and rotating magnetic fields within the formalism of quantum mechanics [1,2]. The probability is a periodic function of the $\sin^2$ type. In NMR, EPR and ODMR the effect is known as Rabi oscillations or transient nutations [3,4].This topic is closely related to the recording, processing, and reading of information using qubits in quantum computing. In 1944 I. I. Rabi received the Nobel Prize for the description and measurement of the magnetic properties of nuclei. In addition to being an outstanding physicist, Isidor Isaac Rabi was also a great humanist. This is evidenced by his book SCIENCE: THE CENTER OF CULTURE , in which, among other topics, he addresses the philosophical problems of science and armaments. He believed that: Science and peace do have a connection. On July 5, 1971, Isydor Izzak Rabi and his wife visited Rymanów. In 2019, twenty years after Rabi's death (January 11, 1988), his wife Margaret Beels, again came to Rymanów with Rabi's four grandchildrens [5].

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Electron Magnetic Resonance in Ni-Mn-Ga-Co-Cu Powders

Łukasz Dubiel [a], Wojciech Maziarz [b], Bogumił Cieniek [c], Ireneusz Stefaniuk [c]

[a] *Rzeszow University of Technology, Faculty of Mathematics and Applied Physics, Department of Physics and Medical Engineering, Powstancow Warszawy 12, 35-959 Rzeszow, Poland*
[b] *Institute of Metallurgy and Material Science Polish Academy of Science, Reymonta 24, 30-059 Krakow, Poland*
[c] *University of Rzeszow, Institute of Materials Engineering, Pigonia 1, 35-959 Rzeszów, Poland*
l.dubiel@prz.edu.pl

Keywords: NiMnGa powder; Heusler alloys; electron magnetic resonance; spin-glass alloy; magnetic properties

Ni–Mn–Ga-based alloys have been widely studied due to the strong coupling between their structural ordering, stoichiometry, and mechanical as well as magneto-mechanical properties [1,2]. Of particular interest is the magnetic-field-induced shape memory effect, first reported by Kari Ullakko [3], which makes these materials promising candidates for functional applications. Although single-crystal Ni–Mn–Ga alloys exhibit outstanding properties, their large-scale industrial use remains limited due to high production costs and technological constraints. Consequently, increasing attention has been directed toward polycrystalline forms, such as melt-spun ribbons and powders, especially in the context of additive manufacturing [4,5].

This poster presents an electron magnetic resonance (EMR) study NiMnGaCoCu powders derived from melt-spun ribbons via mechanical milling. EMR measurements were carried out in the temperature range of 180–380 K during both cooling and heating cycles. Microstructural and compositional characterization was carried out using scanning electron microscopy (SEM) and energy-dispersive X-ray spectroscopy (EDS).

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EPR studies of free radicals and metal ions in silver fir needles and soil

Idalia Kasprzyk [a], Agata Ćwik [b], Katarzyna Kluska [a], Bogumił Cieniek [c], Ireneusz Stefaniuk [c]

[a] *University of Rzeszow, Faculty of Biotechnology, Zelwerowicza 4, 35-601 Rzeszów, Poland*
[b] *University of Rzeszow, Faculty of Technology and Life Science, Zelwerowicza 4, 35-601 Rzeszów, Poland*
[c] *University of Rzeszów, Institute of Materials Engineering, Pigonia 1, 35-959 Rzeszów, Poland*
ikasprzyk@ur.edu.pl

Keywords: free radicals, organics, BPFRs, EPR

Biogenic free radicals (BPFRs) are naturally occurring, stable, and persistent chemical compounds in plants that contain unpaired electrons. They are generated in plants as a result of metabolic processes. BPFRs are present in plant leaves, both in the senescent and active phases. Their concentration increases with plant aging. They can enter the soil from fallen and decaying plant parts, where they interact with soil particles and influence humification processes.

The purpose of this study was to test the hypothesis that the content of biogenic free radicals increases with leaf aging. The study determined the EPR signal of free radicals and metal ions in plant material of varying degrees of aging, as well as in litter, topsoil, and soil sampled at a depth of 5 cm. The samples were collected from five sites located in natural forest ecosystems, in duplicate, with the site located in the city of Rzeszów serving as a control.

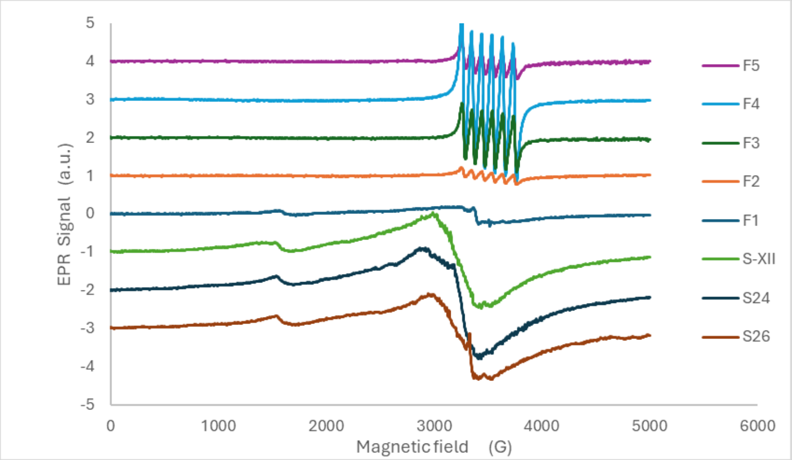

Fig. EPR spectra of samples from a single site: F1 – needle from litter, F2 – young needle, F3 – secondary needle, F4 – tertiary needle, F5 – oldest needle, S-XII – litter, S24 – topsoil, and S26 – soil from a depth of 5 cm.

The EPR spectrum revealed lines originating from Mn^{2+} ions, primarily in needles, and Fe^{3+} ions and free radicals.

This research was supported by the Minister of Science of the Republic of Poland under the Programme „Regional initiative of excellence”. Agreement No. RID/SP/0010/2024/1.

Photocatalytic Activity of H_2O_2–TiO_2(S,C)–HAp/FAp Composites under Visible-Light Irradiation, Studied by EPR

Joanna Kisała [a], Bogumił Cieniek [a], Yaroslav Bobytskyy [b], Ireneusz Stefaniuk [a]

[a] *Institute of Materials Engineering, University of Rzeszow, Pigonia 1, 35-959 Rzeszow, Poland*
[b] *Institute of Physics, University of Rzeszow, Pigonia 1, 35-959 Rzeszow, Poland*
jkisala@ur.edu.pl, bcieniek@ur.edu.pl, ybobytskyy@ur.edu.pl, istefaniuk@ur.edu.pl

Keywords: EPR spectroscopy; S-dopped TiO2; hydroxyapatite; fluoroapatite

Photocatalytic bleaching systems based on TiO_2 are promising for applications in which a reduction of hydrogen peroxide concentration and excitation with visible light are required, for example in biomedical and teeth whitening applications. In this work we investigate the activity of photocatalytic systems of type H_2O_2-TiO_2(S,C)-HAp/FAp under blue (460 nm) and green (525 nm) light irradiation using electron paramagnetic resonance (EPR) spectroscopy with the DMPO spin trap. Spin adduct spectra were recorded in the dark and under illumination to monitor the formation of hydroxyl and superoxide radicals generated from hydrogen peroxide in dimethyl sulfoxide solutions containing nanocrystalline hydroxyapatite and fluoroapatite modified with TiO_2(S,C) and Ag. The radicals were identified, their spectral parameters were determined, and correlations between irradiation conditions and the yields of DMPO OH and DMPO OOH adducts were established. For fluoroapatite-based materials modified with silver and TiO_2, such as Fap-$AgNO_3$ and Fap-TiO_2(S,C), a markedly stronger response to blue light was observed, whereas for pure FAp and samples modified with lutetium, e.g. FAp pure and Fap-AgLu, a higher generation of radicals occurred under green irradiation. The predominance of DMPO OH adducts in many cases is attributed to the transformation of DMPO OOH species, indicating efficient reactive oxygen species formation in these systems. The results demonstrate that H_2O_2-TiO_2(S,C)-HAp/FAp system activated by visible light can generate reactive radicals effectively at reduced H_2O_2 levels, which is advantageous for potential simultaneous bleaching and remineralization applications.

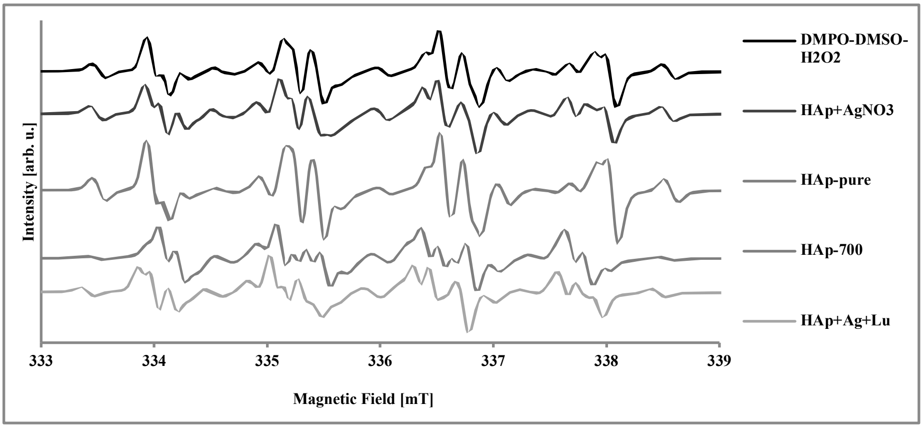

Figure 1. Summarizes the EPR spectra of all samples of hydroxyapatite and spin trap DMPO with the solvent DMSO with H_2O_2 without irradiation.

Application of EPR Spectroscopy for Comparative Analysis of Free Radicals and Paramagnetic Species in House Dust from Rural and Urban Areas

Dariusz Man [a], Barbara Pytel [a]

[a] *Department of Medical Physics, Institute of Physics, Opole University, Oleska 48, 45-052 Opole.*
dariusz.man@uni.opole.pl

Keywords: House dust; EPR spectroscopy; Free radicals.

This paper presents preliminary studies on the correlation between free radicals and paramagnetic species present in house dust and in soil collected from agricultural green areas surrounding residential properties. The results suggest that organic soil is the dominant source of free radicals and paramagnetic ions in house dust, as evidenced by characteristic EPR spectra. This conclusion is further supported by a clear correlation between the shapes of EPR spectra obtained from soil samples and their corresponding house dust samples.

Our findings provide new insights into potential risks to human health, particularly in agricultural regions where organic soils predominate. Interestingly, our study suggests that organic matter, such as humic substances—well-known components of organic soils—may not only constitute a significant source of free radicals but also influence biological systems. Previous studies have demonstrated that these substances can interact with lipid membranes, altering their fluidity, which may have important implications for respiratory health in populations exposed to organic dust. This may help explain the increased incidence of respiratory diseases, such as chronic lung diseases, in rural populations.

EPR and Optical Study of Radiation Effects Induced by Bismuth Ions in Gadolinium Calcium Oxoborate Single Crystals

Ireneusz Stefaniuk [a], Piotr Potera [a], Bogumił Cieniek [a],

[a] *University of Rzeszow, Institute of Materials Engineering, Pigonia 1, 35-959 Rzeszów, Poland*
ppotera@ur.edu.pl

Keywords: oxide crystals, EPR study, optical study.

Gadolinium calcium oxoborate $Ca_4GdO(BO_3)_3$ (GdCOB) crystals are of great interest due to their excellent nonlinear optical properties [1]. GdCOB has the monoclinic noncentro-symmetric structure with two molecules per unit cell and space group symmetry C_m [2].

The EPR measurements were obtained in the temperature range of 95 to 300 K, before and after irradiation by bismuth ions with an energy of 11.4 MeV/u (MeV per nucleon) and a fluence of $5x10^{11}$ cm^{-2} at room temperature. The selected EPR spectra before and after irradiation are presented in Figure 1. The aim of this paper is to determine the nature of the centers produced in the GdCOB crystal after irradiation with bismuth ions. Quantitative analysis of EPR spectra has been carried out using the program EMR_NMR assuming spin Hamiltonian for triclinic site symmetry. The shifting of the fundamental absorption edge and changes in absorption after irradiation will also be studied.

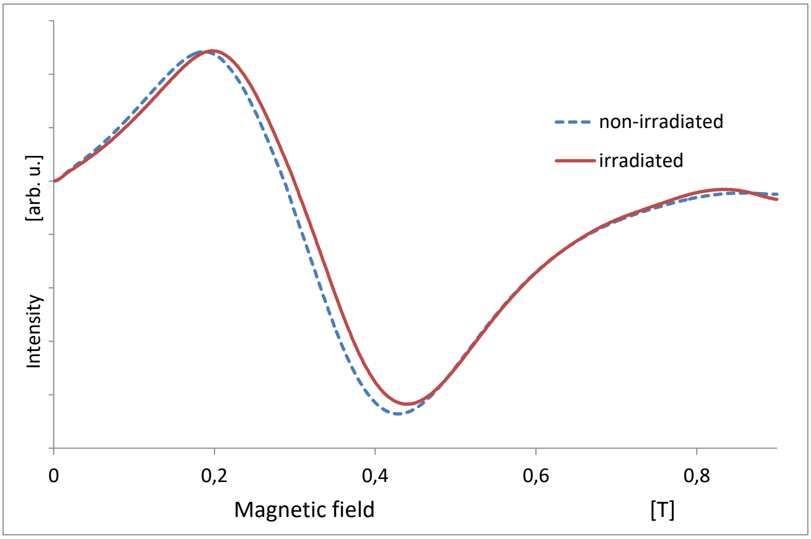

Figure. 1 EPR spectra of GdCOB crystal after and before irradiation with bismuth ions at room temperature at the same orientation

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Analysis of the influence of vanadium complexes on model membranes using electron paramagnetic resonance

Barbara Pytel [a], Dariusz Man [a]

[a] *Institute of Physics, Department of Medical Physics, Opole University, Oleska 48, 45-052 Opole, Poland*
bpytel@uni.opole.pl

Keywords: EPR; vanadium complexes, model membranes, electron paramagnetic resonance, spin probes

Vanadium is present in the human body in trace amounts, yet it is essential for its proper functioning. Vanadium compounds are necessary, among other things, for normal lipid metabolism. They may also play a role in stimulating glucose secretion and glycogen synthesis in the liver. The effectiveness of vanadium depends, among other factors, on the method of administration, the dose used and the duration of exposure. Above all, however, it depends on the oxidation state of vanadium and the type of ligand with which it forms a compound. Excessively high doses of vanadium compounds are toxic to living organisms. Hence, both the carcinogenic and anti-tumor properties of vanadium compounds are being investigated. It is known from the literature that vanadium(IV) acetylacetonate (V4) and vanadium(III) acetylacetonate (V3) stand out from other vanadium compounds due to their high activity and, at the same time, low toxicity. As vanadium complexes affect both diseased and healthy cells, work is underway to incorporate them into liposomes. By ensuring targeted transport of active substances, liposomes protect healthy tissues, reducing the side effects of their action. One of the best methods for studying the effect of biologically active substances on cell membranes is the electron paramagnetic resonance technique, as it allows the dynamics of the membrane to be studied in cross-section.

The aim of this study was to investigate the effect of vanadium(IV) oxyacetylacetonate (V4) and vanadium(III) acetylacetonate (V3) complexes (*Sigma-Aldrich*) on the dynamics of model membranes prepared from dipalmitoylphosphatidylcholine (DPPC) (*Sigma-Aldrich*), as a function of exposure time. In the experiment, the spin probe 2,2,6,6-tetramethylpiperidine-1-oxyl (TEMPO) (*Sigma Aldrich)* was used, which can exist partly in the aqueous environment and partly in the hydrophobic region. Vanadium(IV) complexes were introduced into the aqueous liposome dispersion at ratios of 1% and 2.2% relative to the lecithin. EPR spectra were recorded over 72 h. Analysis of the probe partition coefficient determined from the obtained spectra provided information on the dynamic properties of the membrane under investigation, as a function of the duration of the vanadium(IIII) and vanadium(IV) complex's interaction with the bilayer.

After 72 hours of the experiment, no significant changes in the fluidity of the bilayer were observed under the influence of either the V3 or V4 complex at a concentration of 1%. In contrast, complexes at a concentration of 2.2% caused a slight increase in the surface fluidity of the membrane layer, with this effect being greater in the case of the V4 complex. Furthermore, no significant changes were observed for the V3 complex during the course of the experiment.

Tuning the magnetic coupling in $CoFe_2O_4$-based multishell nanostructures: An EPR spectroscopic investigation

Iwona Rogalska [a], Ireneusz Stefaniuk [a], Bogumił Cieniek [a], Anna Tomaszewska [b], Rober Pązik [b], Magdalena Kulpa-Greszta [b]

[a] *University of Rzeszow, Institute of Materials Engineering, Pigonia 1, 35-959 Rzeszów, Poland*
[b] *University of Rzeszów, Faculty of Biotechnology, Pigonia 1, 35-959 Rzeszów, Poland*
iwrogalska@ur.edu.pl

Keywords: core-shell nanostructures, cobalt ferrite, electron magnetic resonance (EMR), magnetic coupling, anisotropy fields, phase interfaces.

Multishell nanostructures based on ferrimagnetic cobalt ferrite ($CoFe_2O_4$) cores encapsulated by metallic or alloyed shells are crucial building blocks for next-generation spin-polarized data storage, electromagnetic wave absorbers, and advanced biomedical platforms. Their functional performance is predominantly dictated by complex interfacial phenomena within the multishell architecture, where the competition between inter-phase exchange coupling and dipole-dipole interactions plays a key role. In this work, we present a systematic investigation of the temperature-dependent magnetization dynamics, internal magnetic fields, and spin-relaxation mechanisms across a compositional series of core-multishell configurations, designated as $CoFe_2O_4@CoFe_x$ (where $x = 3, 5, 8$). The magnetic properties and phase transitions were probed using temperature-resolved Electron Paramagnetic Resonance (EPR) spectroscopy from room temperature (300 K) up to 451 K at X-band microwave frequency.

At 300 K, all samples exhibit broad, asymmetric, and shifted resonance profiles characteristic of strongly exchange-coupled regimes dominated by large internal fields. However, varying the shell component (x) drastically modifies the line-shape evolution with temperature. For the lower stoichiometry system ($CoFe_2O_4@CoFe_3$), increasing temperature leads to a continuous, monotonic shift of the resonance field toward higher values (centered around 200 mT), accompanied by a substantial narrowing of the linewidth and signal enhancement due to thermally activated reduction in effective magnetocrystalline anisotropy. In sharp contrast, the higher alloy content systems ($CoFe_2O_4@CoFe_5$ and $CoFe_2O_4@CoFe_8$) exhibit a robust, non-zero baseline plateau in the high-field region (> 350 mT) between 300 K and 370 K. This indicates strong spin-pinning effects at the interfacial boundaries of the multishell structure. For $x = 8$, this high-field plateau is thermally stabilized up to 390 K. Only at elevated temperatures (430 K – 451 K) is the local anisotropy barrier overcome, leading to the suppression of the plateau and a sharp growth of the primary resonance peak around 200 mT. These findings demonstrate that tuning the multishell stoichiometry provides a powerful degree of freedom to manipulate interface pinning strength and control spin-lattice relaxation paths.

MBE Growth and Magnetic Characterization of Thin CrTe and CdCrTe Layers

Iwona Rogalska [a], Ireneusz Stefaniuk [a], Bogumił Cieniek [a], Małgorzata Trzyna-Sowa [a], Michał Marchewka [a], Jakub Grendysa [a, b]

[a] *University of Rzeszow, Institute of Materials Engineering, Pigonia 1, 35-959 Rzeszów, Poland*
[b] *CENTERA Laboratories, Institute of High Pressure Physics, Polish Academy of Sciences, Warsaw 01-142, Poland*
iwrogalska@ur.edu.pl

Keywords: MBE, chromium telluride, EPR, SIMS, thin films, zinc-blende structure.

Thin films and low-dimensional structures of chromium telluride (CrTe, CdCrTe) in the metastable zinc-blende (ZB) structure were synthesized via molecular beam epitaxy (MBE) method on hybrid GaAs/CdTe substrates. Technological parameters – including substrate and effusion cell temperatures, alongside Te, Cr and Cd fluxes – were optimized to achieve the target ZB phase under *in situ* RHEED monitoring. Secondary ion mass spectrometry (SIMS) depth profiling confirmed the formation of a well-defined, isolated Cr layer with a thickness of approximately 10 nm.

Electron paramagnetic/magnetic resonance (EPR/EMR) spectroscopy served as the primary diagnostic tool to evaluate the magnetic properties. This method enabled direct analysis of spin-orbit interactions of Cr^{3+} and the determination of their effective g-factor ($g_{eff} \approx 1.98$). Temperature and angular dependent EMR spectra of the CrTe samples revealed distinct variations in the low-field line around 50 mT, clearly indicating magnetic ordering. These findings were compared with reference spectra of CdCrTe (resonance field of 95 mT) as well Cr_2Te_3 samples (resonance fields of 347 mT and 341 mT, solid and powder). With decreasing temperature, of the Cr_2Te_3 resonance line shape transitioned from a Lorentzian profile to a Dyson function. These studies establish a foundation for developing complex quantum structures with CdTe and HgCdTe barriers at the CDNMiN UR.

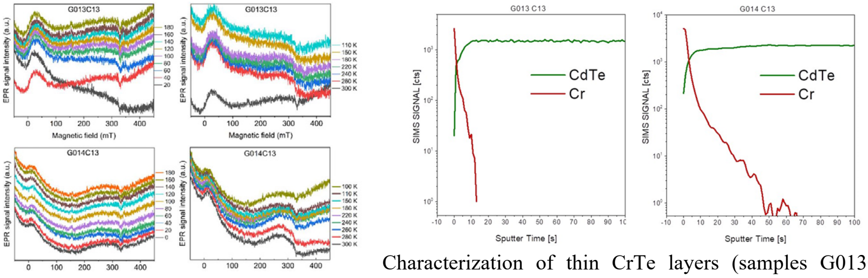

Figure 1. Characterization of thin CrTe layers (samples G013C13 and G014C13) grown by MBE: (left) temperature and angular dependence of electron magnetic resonance (EMR) spectra; (right) SIMS depth profiles showing the distribution of the Cr signal and the CdTe matrix.

Effect of flavanols on the fluidity of the erythrocyte membrane

Izabela Sadowska-Bartosz[a], Grzegorz Bartosz[a], Bogumił Cieniek[b], Ireneusz Stefaniuk[b]

[a] University of Rzeszow, Faculty of Technology and Life Sciences, Institute of Food Technology and Nutrition, Aleksandra Zelwerowicza 4, 35-601 Rzeszów, Poland
[b] University of Rzeszów, Institute of Materials Engineering, Pigonia 1, 35-959 Rzeszów, Poland
isadowska@ur.edu.pl

Keywords: erythrocyte; membrane fluidity; doxylstearic acids; flavanols; catechins

Catechins (monomeric flavanols) and their gallate derivatives are a class of flavonoids mainly present in many plants, and therefore in fruits and vegetables and derived products like fruit juices or jams, Monomeric flavanols are abundant in teas derived from the tea plant *Camellia sinensis*, as well as in some cocoas and chocolates (made from the seeds of *Theobroma cacao*) and wine found in many other plant species. The main catechins present in green tea, as well as in black tea, are (−)-epigallocatechin (EGC) and the ester of epigallocatechin and gallic acid, (−)-epigallocatechin gallate (EGCG).

The aim of this study was to characterize the interaction of chosen catechins erythrocytes as simple model human cells, concentrating on their effect on the membrane structure.

Erythrocyte membranes (2.7 mg protein/mL) were added with catechins to the desired concentrations (0, 50, 100, and 250 μM) and spin-labeled fatty acids, 5-doxyl stearate (5DS) or 16-doxyl stearate (16DS). EPR measurements were performed using microhematocrit capillaries in a Bruker multifrequency and multi-resonance FT-EPR ELEXSYS E580 apparatus operating at the X-band(~9.5GHz employing an ER4119-HS cavity. Flavanols increased the order parameter of membrane lipids and the rotational correlation time τ_c of the probes.

Flavanol	5DS order parameter		
Concentration	Catechin	EGC	EGCG
0	0.610 ± 0.006		
50	0.616 ± 0.007	0.616 ± 0.007	0.616 ± 0.007
100	0.617 ± 0.012	0.617 ± 0.012	0.617 ± 0.012
250	0.618 ± 0.008	0.618 ± 0.008	0.618 ± 0.008
Flavanol	16DS τ_c [ns]		
Concentration	Catechin	EGC	EGCG
0	1.73 ± 0.03		
50	1.62 ± 0.08	1.78 ± 0.005	1.77 ± 0.10
100	1.73 ± 0.28	1.86 ± 0.03**	1.83 ± 0.20
250	1.81 ± 0.15	1.99 ± 0.23	1.79 ± 0.01*

As the doxyl group of 5DS is located close to the membrane surface, and that of 16DS in the hydrophobic core of the membrane, these results demonstrate that flavanols increase membrane rigidity both in the polar and in the hydrophobic region.

EPR spin trapping study of radical formation by indocyanine green: influence of aggregation and albumin binding

Magdalena Szpunar[a], Łukasz Dubiel[b], Bogumił Cieniek[c], Ireneusz Stefaniuk[c],
David Aebisher[d], Andrzej Wal[e]

[a]Doctoral School at the University of Rzeszów, Tadeusza Rejtana 16C, 35-959 Rzeszów, Poland
[b]Rzeszów University of Technology, Department of Physics and Medical Engineering, Faculty of Mathematics and Applied Physics, Powstanców Warszawy 12, 35-959 Rzeszów, Poland
[c]University of Rzeszów, Institute of Materials Engineering, Faculty of Exact and Technical Sciences, Pigonia 1, 35-310 Rzeszów, Poland
[d]University of Rzeszów, Department of Photomedicine and Physical Chemistry, Faculty of Medicine, Warzywna 1A, 35-310 Rzeszów, Poland
[e]University of Rzeszów, Institute of Physics, Faculty of Exact and Technical Sciences, Pigonia 1, 35-310 Rzeszów, Poland
magdalenaszp@dokt.ur.edu.pl

Keywords: indocyanine green (ICG), electron paramagnetic resonance (EPR), spin trapping, reactive oxygen species (ROS), photodynamic therapy (PDT), hydroxyl radicals

Reactive oxygen species (ROS) generated during photodynamic therapy (PDT) play a key role in oxidative damage of cancer cells. In type I PDT mechanisms, electron transfer processes lead to the formation of radical species such as superoxide and hydroxyl radicals, which are particularly important under hypoxic conditions. Indocyanine green (ICG), a clinically approved near-infrared dye, has recently attracted considerable attention as a potential photosensitizer due to its favorable photophysical properties and strong affinity toward serum albumin.

In this work, electron paramagnetic resonance (EPR) spin trapping spectroscopy was used to investigate radical species generated by ICG under light irradiation. Experiments were performed for aqueous ICG solutions at concentrations of 55 μM and 160 μM, both in the absence and presence of bovine serum albumin (BSA). Radical intermediates were detected using the spin trap DMPO and EPR spectra were analysed using hyperfine splitting constants and EasySpin simulations.

The dominant contribution originated from the DMPO-OH adduct, indicating efficient hydroxyl radical formation consistent with a type I photodynamic pathway. Quantitative analysis of EPR signal intensities revealed that both dye concentration and albumin binding significantly affect radical generation kinetics. UV-Vis measurements confirmed concentration-dependent aggregation of ICG and showed that BSA stabilizes the monomeric form of the dye.

The results demonstrate that aggregation and protein binding strongly influence the photodynamic activity of ICG and radical formation pathways. These findings may contribute to a better understanding and optimization of ICG-based photodynamic systems.

Optical, Structural and Magnetic Properties of Chromium-Doped Titanium Oxide Thin Films Deposited by Reactive DC Magnetron Sputtering

Grzegorz Wisz [a], Piotr Potera [a], Ireneusz Stefaniuk [a], Bogumił Cieniek [a], Dariusz Płoch [a]

University of Rzeszów, Institute of Materials Engineering, Pigonia 1, 35-959 Rzeszów, Poland
gwisz@ur.edu.pl

Keywords: titanium oxide, chromium doping, magnetron sputtering, thin films, magnetic properties.

Chromium-doped titanium oxide (TiO_2:Cr) thin films were deposited on glass and silicon substrates by reactive DC magnetron sputtering under different oxygen partial pressures and chromium concentrations. The influence of deposition parameters on the structural, optical and magnetic properties of the obtained films was investigated. X-ray diffraction analysis confirmed the formation of nanocrystalline TiO_2 films with the incorporated chromium ions affected the crystallite size and induced lattice distortions. Surface morphology studies revealed homogeneous and compact coatings with good adhesion to the substrate. Optical measurements performed using UV–VIS spectroscopy indicated high transparency in the visible range and a gradual reduction of the optical band gap with increasing chromium content. The observed band gap narrowing is associated with the introduction of localized electronic states related to Cr ions within the TiO_2 band structure. Magnetic characterization demonstrated weak room-temperature ferromagnetic behavior for selected TiO_2:Cr films, suggesting the possibility of tailoring magnetic ordering through dopant concentration and deposition conditions. The obtained results demonstrate that reactive DC magnetron sputtering is an effective method for producing multifunctional TiO_2:Cr thin films with tunable optical and magnetic properties, which may be promising for applications in spintronics, optoelectronics, photovoltaics and photocatalytic systems.

Assessment of the Safety of Physiotherapeutic Laser Therapy on Tattooed Skin Using EPR Spectroscopy

Wojciech Żyłka [a], Barbara Pilch-Pitera [b], Renata Skalska-Izdebska [c], Ireneusz Stefaniuk [a]

[a] University of Rzeszow, Institute of Materials Engineering, Pigonia 1, 35-959 Rzeszów, Poland
[b] Rzeszów University of Technology, Faculty of Chemistry, Powstańców Warszawy 6, 35-029 Rzeszów, Poland
[c] State University of Applied Sciences in Przemyśl, Institute of Health Protection, Książąt Lubomiskich 4, 37-700 Przemyśl, Poland
wzylka@ur.edu.pl

Keywords: EPR spectroscopy, tattoos, tattoo pigments, high-energy therapeutic laser

The study evaluated the effect of high-energy laser radiation, commonly used in physiotherapeutic treatments, on selected tattoo inks. The aim of the research was to determine whether laser exposure may induce the formation of free radicals in tattoo pigments, which could be relevant to the safety of laser procedures performed on tattooed skin. Electron paramagnetic resonance (EPR) spectroscopy was employed to detect paramagnetic and radical centers. Ink samples containing various pigments, including carbon black, iron oxide black, titanium white, phthalocyanine green, phthalocyanine blue, monoazo yellow, monoazo orange, naphthol red, and madder dye, were exposed to a high-energy laser under conditions corresponding to real physiotherapeutic treatments. The EPR signals recorded before and after laser irradiation were subsequently compared. Particular attention was devoted to the potential generation of free radicals, which in biological environments may react with proteins and nucleic acids, including DNA, potentially leading to genetic material damage and changes associated with mutagenic effects. The findings of this study may contribute to the assessment of the safety of laser therapy procedures in individuals with tattoos.

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