

Habilitációs pályázati anyag

Tartalomjegyzék / [Table of contents](#)

I. LEÍRÓ SZAKMAI ÖNÉLETRAJZ és KUTATÁSI TERV / NARRATIVE CV and RESEARCH PLAN	2
II. SZAKMAI ÖNÉLETRAJZ / CURRICULUM VITAE	6
III. TUDOMÁNYMETRIAI ADATOK / SCIENTIFFIC METRICS:	9
ELŐZŐ 5 ÉV 5 LEGFONTOSABB KÖZLEMÉNYE / 5 MOST IMPORTANT PUBLICATIONS FROM THE LAST 5 YEARS	10

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Félvezető Nanoszerkezetek “Lendület” kutatócsoport

Szilárdtestfizikai és Optikai Kutatóintézet

HUN-REN Wigner Fizikai Kutatóközpont

Kutatócsoportvezető: Gali Ádám

I. LEÍRÓ SZAKMAI ÖNÉLETRAJZ és KUTATÁSI TERV / NARRATIVE CV and RESEARCH PLAN

Személyes adatok / Personal details

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Summary of Scientific Career

I began my academic journey as a first-generation university student, eventually becoming a researcher with a focus on nanoscience, materials engineering, and quantum technology. My research career started with surface analysis techniques, including X-ray photoelectron spectroscopy and secondary ion mass spectroscopy, during my undergraduate years. This foundation led me to explore surface reactions, exotic nanosystems, and quantum physics.

One of my early achievements was describing the reaction of CO gas with silicon surfaces, resulting in the formation of SiC nanocrystals with shape variations depending on surface orientation. I developed a nucleation and growth model explaining the surface-dependent shapes and nucleation density of these nanocrystals, facilitating the stress-free growth of SiC layers on silicon through a patented method.

My work with SiC drew the attention of Adam Gali, a theoretical expert in the field, leading to our collaboration at the Wigner RCP, where we established a group that integrated experimental and theoretical approaches. During my PhD studies, I focused on SiC quantum dots, building an experimental laboratory and research team that engaged over 20 students. The Gali group now includes eight members in the experimental working group, with four PhD students, and three physicists. I directly supervise two PhD students and a postdoc, while advising the others. I also led two laboratories at the Wigner ADMIL infrastructure and the quantum optical laboratory until relocating my primary research to Notre Dame.

I leveraged my expertise in SiC to address real-world applications, particularly in tuning the optical properties of SiC quantum dots through surface science. I also developed methods for SiC nanoparticle synthesis and pore formation across all SiC polytypes and other semiconductors. Collaborative efforts demonstrated the potential of SiC nanoparticles in biomedical and electronic applications, such as two-photon microscopy probes and immune response triggers, which could lead to guided bone formation and memory device construction.

Recognizing the optical limitations of SiC due to its large bandgap, I worked on color center formation in SiC nanoparticles, culminating in the realization of divacancy quantum bits in 4 nm SiC nanoparticles. This research led to my role as a research fellow at HUN-REN Wigner RCP, where I helped design and establish the quantum optical laboratory, now equipped to study solid-state color centers in various materials, with a focus on quantum computing and quantum information processing.

To further my research, I joined the Stavropoulos Center for Complex Quantum Research at the University of Notre Dame, where I am currently learning about condensed matter physics and quantum material synthesis under the guidance of Profs László Forró, Nirmal Ghimire, and Budih Assaf. The University of Notre Dame has also provided me with opportunities to enhance my skills in teaching, project management, outreach, and leadership through various training programs.

An NIH-funded project inspired my next research focus. This collaborative effort aimed to enhance photoimmunotherapy, a promising cancer treatment limited by light penetration issues. Although SiC nanoparticles showed promise, they were not efficiently excitable by X-ray to produce visible photons. I quickly developed a new system based on Cr-doped ZnGa₂O₄, which proved effective. The properties of spinel structures became the basis for my next career pursuits.

X-ray-mediated therapy and theranostics offer significant promise for advancing future treatment methods. Motivated by this potential, I formed a consortium with Giancarlo Salviati and successfully secured funding through the EU Horizon EIC-Pathfinder program. As Principal Investigator of the PERSEUS project, my goal is to develop a novel cancer treatment approach based on computer tomography, utilizing a complex nanosystem composed of TMDCs, gold, organic sensitizers, and micelle structures.

Both SiC and scintillators-based research made necessary at some point to specify our measurement capabilities for further development. Through the QNL funding, I designed, and built an integrating sphere-based ODMR setup, with contribution of PhD students and a postdoc. This apparatus enables the measurement of optical properties in ensembles of optical defects, with the high-power laser providing excitation over a large area. This approach mitigates inconsistencies arising from the inhomogeneity of powder samples typically encountered in confocal setups. Additionally, for our scintillator studies, we developed a system capable of comprehensive optical measurements—including photon emission, UV-Visible spectroscopy, and imaging—under X-ray excitation.

Future plan

Returning to Wigner RCP, I plan to deepen my research in the synthesis and analysis of scintillators and spinel structures. The synthesis of high-quality bulk crystals, thin films, and nanostructures is crucial for advancing quantum materials research. While the scientific value of a material is closely tied to its physical properties, achieving the necessary material quality is often challenging due to the limitations of scalable synthesis techniques designed primarily for fundamental physics research. My research aims to bridge this gap by translating fundamental discoveries into practical solutions that address both domestic and global social and environmental challenges. In the short term, my work will focus on two key areas: the fundamental understanding and application of spinel structures and the emerging field of introducing chirality to inorganic crystalline materials.

The magnetic and electronic properties of transition-metal compounds are profoundly influenced by crystal-electric field (CEF) splitting of d-electron energy levels, which is highly dependent on the symmetry of the surrounding electric field. Spinel, known for their significant electrical and magnetic properties, hold considerable technological importance. Many spinels exhibit insulating ferrimagnetism with high saturation magnetization and magnetic-ordering temperatures, making them promising candidates for applications in spintronics, spin-caloritronics, nonvolatile memories, and microwave technologies. Additionally, spinels can display ferro- or antiferromagnetism, with complex magnetic behaviors such as Néel, Yafet–Kittel, and spin-spiral ground states. Recent research has also explored altermagnetism in spinels. Some spinels exhibit unconventional spin-relaxation behavior, similar to spin-spin relaxation in two-dimensional triangular lattice antiferromagnets. For instance, studies on CdCr_2X_4 compounds have shown that lattice distortion stabilizes coplanar magnetic order, introducing chirality through the lack of inversion symmetry and triggering a magnetic transition.

Chirality, defined by the inability to superimpose an object onto its mirror image, is a fundamental symmetry in biomolecules and drugs. Natural processes like photosynthesis, which efficiently convert solar energy into chemical energy, rely on chiral Mg-porphyrin complexes. Spinel systems, particularly 3d transition-metal oxides, are effective catalysts for oxygen evolution and photocatalysis. Their optical properties, including photoluminescence and magneto-optical recording, make them versatile for applications in scintillation. Scintillators, which emit photons upon excitation by high-energy particles, have potential applications in X-ray-induced photodynamic therapy (X-PDT), X-ray-induced phot-immunotherapy (X-PIT), drug delivery systems, and anti-counterfeiting technologies—areas in which I am currently engaged. I believe that introducing chirality to these systems will significantly enhance their efficiency and applicability.

In the next year, my primary focus will be on the PERSEUS project, which lasts until mid-2027. Our primary tasks are the development of an analytical method for selectively tracking different types of reactive oxygen species (ROS) under X-ray excitation and describing the underlying processes. I have recruited an experienced postdoctoral researcher for PERSEUS, Árpád Jakab, who has expertise in theoretical modeling, X-ray, and optical systems, making him ideal for this project. With his and Gábor Bortel's assistance, we have already simulated real-life systems (cell and body models) and made significant strides in the experimental characterization of nanosystems with the participation of two graduate students. I am confident that the capability for simultaneous X-ray and visible spectroscopic characterization of nanomaterials holds vast potential, especially as the use of X-rays in everyday life, patient care, and research is expanding. The results from the PERSEUS project hold the promise of a new type of cancer treatment. Although this is a high-risk, high-gain project—as expected from an EIC Pathfinder grant—X-ray-mediated therapy is highly researched in other contexts, but the material responses are less understood. For example, the probes used for ROS are found to be sensitive to X-rays, making the determination of the exact amount of ROS a challenge we aim to solve.

While PERSEUS focuses on measurement and modeling, with materials developed by our collaborators, the spinel-based scintillator development under a "TKP" project is currently ongoing. In the next three years, I intend to continue this research and gradually transition into chiral crystal growth. Currently, our research centers on ZnGa_2O_4 -based scintillators, where the optical properties are highly influenced by deviations from the stoichiometric ratio in the precursor for Mn doping but not for Cr. This makes the synthesis challenging but provides an opportunity for fine-tuning the emission properties, including wavelength and emission time. Our NIH project previously failed to demonstrate the activation of the PIT dye through X-ray excited optical emission; however, our current results may make this possible, representing a breakthrough in cancer research. Utilizing the outcomes of the PERSEUS project, we will be able to explore and precisely measure the efficiency of X-ray-induced photodynamic therapy (X-PDT) on our nanocrystals, and I believe these results will foster new collaborations.

Besides application-oriented research, I aim to understand crystal formation under hydrothermal conditions and the physics behind the optical properties of the studied spinel oxides. The emission of the dopants is influenced by neighboring defects—such as antisite vacancies, vacancy pairs, and oxygen vacancies—which can shift emission wavelengths and alter luminescence times. Doped spinels are known for their long-lasting luminescence, attributed to the presence of exciton traps. Not only are these exciton traps not yet identified, but the relaxation processes—and therefore the long-lasting photoluminescence (LLP) time—are highly dependent on the types of complex defects formed from the dopant and nearby point defects. We have demonstrated that the phenomenon is much more complex than previously thought, with interactions occurring between different complex defects. A more precise description requires further research.

These research endeavors rely on the robust optical characterization capabilities and extensive X-ray research experience of the Institute of Solid State Physics and Optics at the HUN-REN Wigner Research Centre for Physics. We have extensive facilities for material synthesis in the Wigner ADMIL. With recent developments, optical characterization is also feasible, thanks to the various systems we have developed. However, I anticipate that strong collaborations will be essential for comprehensive material characterization. Collaboration with Dr. Gábor Bortel and access to X-ray beam facilities are crucial for my research.

My short-term plans in the Centre relay on the ongoing project, I lead or being involved. Those project cover both, fundamental and applied research. My long-term vision is to establish a group which become the leader in optically active materials, specialized in enantioselective synthesis of chiral structures. I possess expertise in nanomaterial synthesis and have recently begun studying single-crystal growth. I believe that the production of high-quality single crystals will become essential, particularly for advancing fundamental research. Therefore, I plan to expand my knowledge and collaborate with my colleagues, who have decades of experience in single-crystal growth, to synthesize doped spinel oxide crystals. Since achieving enantioselective growth to produce crystals of a nano, or single chiral form is non-trivial, even using chiral organic molecules or biomolecules as structure-directing agents that can induce chirality during crystal growth, I will focus on the realization of such synthesis. On the other hand, the further developments are needed for characterization. I am planning, to expand our optical setups with circular dichroism and birefringence measurement capabilities to use optical studies for material characterization – for single crystals and for the capability of the measurement of light polarizability, which have the potential to enhance light matter interaction in life sciences, catalysis, and other fields

The short-term plans at the Centre focus on the ongoing projects I lead or am involved in, encompassing both fundamental and applied research. These projects lay the foundation for my long-term vision: to establish a research group that becomes a leader in optically active materials, specializing in the enantioselective synthesis of chiral structures.

I possess expertise in nanomaterial synthesis and have recently begun studying single-crystal growth. I recognize that the production of high-quality single crystals is essential, particularly for advancing fundamental research in materials science and quantum technologies. Therefore, I plan to expand my knowledge and collaborate with colleagues who have decades of experience in single-crystal growth to synthesize doped spinel oxide crystals. Achieving enantioselective growth to produce crystals at the nanoscale or in a single chiral form, however, is a significant challenge, even when employing chiral organic molecules or biomolecules as structure-directing agents to induce chirality during crystal growth. I will focus on realizing such synthesis through solvothermal synthesis.

Further advancements in characterization techniques are necessary to fully understand and optimize these chiral materials. I plan to enhance our optical setups with capabilities for circular dichroism (CD) and birefringence measurements. CD spectroscopy will allow us to determine enantiomeric excess and study electronic transitions sensitive to chirality, while birefringence measurements will provide insights into anisotropic optical properties essential for understanding light-matter interactions. By implementing these techniques, we can perform comprehensive optical studies for material characterization—both for single crystals and for measuring light polarizability—which have the potential to enhance applications in life sciences, catalysis, and other fields.

I know, however, that the key connection to the mission of the Institute extends beyond materials science to quantum technology. The phenomenon of chirality-induced spin selectivity (CISS) has garnered increasing attention due to its influence on electron spin polarization along the direction of momentum. In chiral systems, the CISS effect leads to significant spin polarization without the need for external magnetic fields, which has profound implications for spintronic devices and quantum computing.

Chiral organic and inorganic crystals with topological quantum properties present promising applications that warrant further exploration. For instance, spinel structures doped with specific transition metals can exhibit both chiral symmetry and topologically protected electronic states. This research aligns closely with the main focus of the Institute, and by continuing my collaboration with the Gali Group, Levente Rózsa, and others, we can advance the study of spinel structures for quantum technology applications. A more detailed plan for this research field—particularly concerning the experiments and necessary instrumentation—is currently being developed and will be part of my ERC application. Direct experimental determinations of the CISS effect largely fall into two main measurement modalities: Spin-Dependent Electron Transport Measurements and Spin-Polarization Measurements Induced by Charge Polarization. To measure the CISS effect, spin-resolved XPS: ARPES) can be used in facilities such as the APE beamline at Elettra, we can directly measure the spin polarization of electrons emitted from chiral crystals, probing the electronic band structure and spin textures associated with topological states. The new XPS-UPS setup at the Center for Energy Research enables the study of valence band structures and work functions, providing complementary information to XPS and ARPES. I am interested in time resolved ESR and mc-AFM measurement I am looking for collaborations both in and out of the Centre. The increasing number of reviews and recent articles in the field underscores not only its potential significance—which could enhance the Centre's reputation through early contributions—but also highlights the critical importance of carefully designed experiments. Although the CISS phenomenon was first observed in transport measurements, the presence of metal leads, magnetic fields, and complex interfaces often complicates interpretation. By focusing on surface-sensitive, and contactless techniques and high-quality chiral crystals, we aim to obtain high quality research in this field.

Competencies

My research spans a broad spectrum of scientific disciplines, focusing on interdisciplinary studies that integrate materials science, chemistry, quantum technology, life sciences, and engineering. This work is underpinned by a strong foundation in both experimental techniques and theoretical understanding, enabling the precise synthesis and characterization of advanced materials.

Spectroscopic techniques are central to my research interests. However, I acknowledge that some of them are highly specialized techniques, and I cannot say I am an expert in any of them. I aspire to build a research group instead, that includes experts in these areas to further enhance our capabilities. As a materials scientist, I specialize in harnessing these techniques—particularly in combination—for materials development and fundamental understanding. This is demonstrated by the development of the No Photon-Excitation Generation Chemistry (NPEGEC) theory, where the successful measurement of weak chemiluminescence under harsh conditions, application of redox reactions, and detailed analyses using TEM, photoluminescence PL, and UV-Vis absorbance led to the construction of a new reaction theory. More recently, we have described some unusual properties of MXenes, facilitated by guided studies involving XRD, magnetic susceptibility measurements, microwave resistivity, ESR, XPS, and heat capacity analyses. I have had the opportunity to collaborate with experts proficient in these techniques. When the studied systems are complex and imperfect—as is often the case with nanomaterials—individual techniques may only provide partial insights. My competence lies in integrating data from diverse techniques to develop a comprehensive understanding, which can be

challenging for specialists focused on a single field. In our unpublished work, I propose the presence of titanium suboxides responsible for the anomalies in the material around room temperature. The presence of this phase is undoubtedly not detectable with XRD; however, thanks to the phase transitions of these materials, the combination of the aforementioned measurements unravels the presence of such phase.

Furthermore, I have significant expertise in nanoparticle synthesis, particularly using high-pressure reactor systems. During my Ph.D., I developed a method for the high-yield synthesis of ultrasmall silicon carbide (SiC) nanoparticles. Later, I demonstrated the possibility of realizing emission centers in SiC nanoparticles through chemical synthesis. Building on this experience, I developed the synthesis of chromium-doped gallate nanoparticles and SiC-gallate core-shell systems.

I am certain that this technique allows for the production of high-quality and high-yield nanoparticles and even larger single crystals. Hydrothermal synthesis plays a pivotal role in my research, offering a versatile and scalable method for producing nanomaterials with controlled size, morphology, and crystallinity. This technique involves conducting chemical reactions in solutions at elevated temperatures and pressures, typically within sealed autoclaves. The high-pressure environment facilitates the formation of crystalline phases that are difficult to achieve under standard conditions. For example, in the synthesis of spinel oxide nanoparticles, hydrothermal methods enable precise control over doping levels and particle size, which are crucial for tailoring their optical properties. Moreover, the hydrothermal method is environmentally friendly, often using water as the solvent and eliminating the need for organic solvents or high-energy inputs. It also enables the synthesis of metastable phases and nanostructures with unique properties, which are invaluable for advancing research in quantum materials and photonic applications.

II. SZAKMAI ÖNÉLETRAJZ / CURRICULUM VITAE

Current Positions:

- 2024 – Current senior lecturer – tenure-track, Óbuda University, Kandó Kálmán Faculty of Electrical Engineering, Budapest, Hungary
- 2022 – Current: Postdoctoral Research Fellow, Stavropoulos Center for Complex Quantum Matter, Notre Dame, IN, USA
- 2011 – Current: Assistant Research Fellow, Research Fellow, HUN-REN Wigner Research Centre for Physics, Institute of Solid State Physics and Optics, Budapest, Hungary

Previous Positions:

- 2019 – 2022: Budapest University of Technology and Economics, Department of Atomic Physics, (research fellow)
- 2013 – 2015: Visiting Assistant lecturer, University of Pécs, Pécs, Hungary
- 2012 – 2015: Budapest University of Technology and Economics, Department Chemical Engineering and Bioengineering (TA)
- 2008 – 2010: Intern Institute of Technical Physics and Materials Science, Centre for Energy Research, Budapest, Hungary
- 2006 – 2008: Intern Budapest University of Technology and Economics, Faculty of Natural Sciences, Budapest, Hungary

Education

- 2022 Postdoctoral studies, Physics and Leadership, University of Notre Dame, Notre Dame
- 2017 PhD, chemistry, Budapest University of Technology and Economics, Budapest, Hungary
- 2013 NanoValid Training and Workshop University of Zaragoza, Zaragoza, Spain
- 2012 XIX International Summer School Fluorescent Nanoparticles in Biomedicine Instituto Universitario de Ciencia de Materiales, Madrid, Spain
- 2010 Diploma (MSc), Chemical Engineer, Budapest University of Technology and Economics

Research Experience

Fellowships and Awards (Selected)

- János Bolyai Research Fellowship from the MTA (2019-2022)
- UNKP New National Excellence program (2019-2020, 2020-2021, 2021-2022)
- NTP-NFTÖ-18,16, NTP-EFÖ-P15 National Talent Programs (3 times)
- Research Student Bursary – E-MRS2014
- TÁMOP 4.2.4. A/2-11-1-2012-0001 „National Excellence Program 2013-2014.
- National Traveling grants: MTA 2017/I, 2018/I Wigner: 2018/I 2016/I, 2014/I,II, 2013/I (MTA is the Hungarian Academy of Sciences)
- György Ferenczi memorial award for semiconductor research (2020)
- Hungarian Academy of Sciences Early Career Researcher Award (2019)
- BME Research Grant (2017) (Budapest University of Technology and Economics)
- Graduate Student Award (GSA) E-MRS Lille 2016

Supervision of Graduate Students and Postdoctoral Fellows

2016 – Present: 5 MSc and 1 BSc students, 2 PhD students, 1 Postdoc

2011 – 2016: Advisor of 2 BSc and 7 MSc students

Teaching Activities

2022 – 2024	University of Notre Dame, IN, USA
2019 – 2022	Department of Atomic Physics, Budapest University of Technology and Economics
2013 – 2015	University of Pécs, Hungary:
2012 – current	Department of Chemical Engineering and Bioengineering Budapest University of Technology and Economics

Organization of Scientific Meetings

- COSE-JAM Research Horizons 2023, Notre Dame, IN, USA
- “kvantumtech” Seminar Series, BME 2018-2022

Institutional Responsibilities

2024:	Member of the ND Nano Leadership Team, University of Notre Dame,
2020 – 2022:	deputy leader of the Fit4Nano Hungarian contribution
2019 – 2022:	Seminar Organizer, Budapest University of Technology.
2018 – 2022:	Leader of the Quantum Optical Laboratory, HUN-REN Wigner RCP
2016 – 2022:	deputy leader of the WIGNER ADMIL, HUN-REN Wigner RCP
2016 – 2022:	Leader of the Colloid Laboratory HUN-REN Wigner RCP
2023 – current:	Member of the Diversity Committee, University of Notre Dame
2022 – 2023:	President of the Work Council, HUN-REN Wigner RCP
2022 – current:	Member of the Work Council, HUN-REN Wigner RCP
2023 – current:	Member of the Diversity Committee, HUN-REN Wigner RCP

Invited Talks

- Size Selective Optical and Photocatalytic Properties of Silicon Carbide Nanoparticles 7th Global Conference on Materials Science and Engineering (CMSE 2018) Xi’an, China Aug 21-24, 2018
- Enhancement of Red X-Ray Excited Luminescence of Chromium Doped Zinc Gallate by Ultrasmall Silicon Carbide Nanocrystals, E-MRS Spring Meeting and Exhibit, virtual, May 25-29. 2020
- Enhancement of Red X-Ray Excited Luminescence of Chromium Doped Zinc Gallate by Ultrasmall Silicon Carbide Nanocrystals, E-MRS Spring Meeting and Exhibit, virtual, May 25-29. 2021

- Enhancement of Red X-Ray Excited Luminescence of Chromium Doped Zinc Gallate by Ultrasmall Silicon Carbide Nanocrystals, Global Virtual Conference on Nanotechnology, virtual, June 22. 2021.
- The applications of and need for a complex understanding of the silicon carbide nanosystems, NDnano network meeting, June 12. 2023. Notre Dame, IN, USA
- Microstructure-Dependent Optical Properties of Doped Spinel Oxide Nanosystems, APS March Meeting, March 5-10. 2023., Las Vegas, NV, USA

Outreach

Researcher's Night
Quantum tech seminars

APS Public Engagement team
APS Career Mentoring Fellow, 2024
Notre Dame Science Olympiad
COSE-JAM science day for undergraduate students
Northern Indiana Science and Engineering Fair

Received fellowships and grants

2023 – 2027 HORIZON-EIC-2022-PATHFINDEROPEN-01-01 101099423
PERSEUS PERSEUS-2D Material-Based Multiple Oncotherapy Against
Metastatic Disease Using a Radically New Computed Tomography
Approach (301k €)

2023 –2024 APS Career Mentoring Fellow, 2024

2021 – 2022 Quantum Information National Laboratory: *Quantum Optical System
development for inspection of bulk quantum-coherent materials,
Synthesis of Quantum Nano-Objects* (179k €/Y)

2019 – 2022 János Bolyai Research Fellowship from the MTA

2019 – 2022 New National Excellence Program: Synthesis and Characterization of
optical defects in Silicon Carbide Nanoparticles (8,000 €/Y)

2015, 2016-2018 National Talent Program (2000 €/Y)

2013 – 2014 National Excellence Program (6000 €/Y)

Travel Grants

Research Student Bursary – E-MRS2014
National Traveling grants: MTA 2017/I, 2018/I Wigner: 2018/I 2016/I, 2014/I,II, 2013/I

Contribution to Scientific Projects as WP, Task or Delivery Leader

2021- current MTA establishment fund (Momentum program): *Design and characterization
of semiconductor nanostructures for biomarker, solar cell and
magnetometer applications*

2012-2016OTKA No. K101819: *Design, fabrication and analysis of luminescent silicon
carbide nanocrystals for in vivo biomarker applications*

2012-2016OTKA No. K106114: *Development of novel silicon carbide nanomarkers and
more effective glutamate and GABA uncaging materials for measurement
of neuronal network activity and dendritic integration with three-
dimensional real-time two-photon microscopy*

2016-2019Visegrad Group (V4) + Japan Joint Research Project on Advanced Materials:
*Nanophotonics with metal - group IV-semiconductor nanocomposites:
From single nanoobjects to functional ensembles (NaMSeN)*

2016-2019 NVKP_16-1-2016-0043: *Development of fluorescent dyes and microscope for the
treatment of epilepsy*

2017-2021NKFIH Grant No. 2017-1.2.1-NKP-2017-00001: *National Quantumtechnology
Program: Creation and distribution of quantum bits and development of
quantum information networks*

2019-2023 National Excellence Program: *Quantum-coherent materials***III. TUDOMÁNYMETRIAI ADATOK / SCIENTIFIC METRICS:**

(Based on MTMT)

Publication types	Count		Citation ¹	
	All	Detailed	Independent	All
I. Scientific journal articles	<u>22</u>			
in international journal in foreign language		<u>22</u>	<u>315</u>	<u>452</u>
Effective citations			255.25	
Since 2017 (PhD)			174	
II. Books	0			
III. Book chapter	0			
IV. Conference in journal or conference paper	<u>3</u>			
in foreign language		<u>2</u>	0	0
in hungarian		<u>1</u>	0	0
Publications (I-IV.)	<u>25</u>		<u>315</u>	<u>452</u>
Abstract³	<u>5</u>		0	0
Research data	0		0	0
Other scientific works⁴	<u>7</u>		0	0
All scientific publications	<u>37</u>		<u>315</u>	<u>452</u>
Hirsch index⁵			<u>10</u>	<u>12</u>
Achievements	0		0	0
Popular science works	<u>1</u>			
Journal articles		<u>1</u>	0	0
Of public interest or unclassified publications⁶	0		0	0
More publications⁷	0		0	0

Other authorships⁸	0		0	0
Citations of edited publications			0	0
Citations in dissertations and other types			<u>20</u>	<u>22</u>
All publications and citations	<u>38</u>		<u>335</u>	<u>474</u>

Scientific publications	after getting (PhD 2017)	All
1.0 All publications count	<u>12</u>	<u>25</u>
1.1 Publications in SCI referred journals	<u>12</u>	<u>22</u>
Mailing author	<u>4</u>	<u>14</u>
Single author	0	0
First author		13
Last author	1	1
1.2 Publications in hungarian journals	0	0
1.3 Number of given basic patents	0	0
1.4 Publications in other international journals	0	0
1.5 Publications in other Hungarian journals	0	0
1.6 In proceedings (proceedings: complete work)	0	<u>3</u>
1.7 Summary works	0	0

Scientometrics	i,H
Citations of all theses, without self-citations	<u>315</u>

Special Data	Data	percentage of all
The last scientific degree (PhD 2017) number of publications	<u>12</u>	---
Number of publications published in Hungarian and their percentage of all	<u>1</u>	4%
The number of citations of the top five publications with the highest independent citation count. ³	<u>174</u>	---
Hirsch-index ³	<u>12</u>	---

Scientific publications	after getting (PhD 2017)	All
Cumulated Impact factor	<u>76.717</u>	<u>120.172</u>
No. of D1 articles	<u>9</u>	<u>14</u>
No. of Q1 articles (without D1)	<u>5</u>	<u>8</u>

Scientometrics	i,H
Citations of all thesis, without self citations	<u>315</u>

Special Data	Data	percentage of all
The last scientific degree (PhD 2017) number of publications	<u>12</u>	---
Number of publications published in Hungarian and their percentage of all	<u>1</u>	4%
The number of citations of the top five publications with highest independent citation count. ³	<u>174</u>	---
Hirsch-index ³	<u>12</u>	---

ELŐZŐ 5 ÉV 5 LEGFONTOSABB KÖZLEMÉNYE / 5 MOST IMPORTANT PUBLICATIONS FROM THE LAST 5 YEARS

1. Ultrahigh nitrogen-vacancy center concentration in diamond *Sándor Kollarics, F Simon, András Bojtor, Kristóf Koltai, Gergely Klujber, Máté Szieberth, Bence Gábor Márkus, David Beke, K Kamarás, A Gali, D Amirari, R Berry, S Boucher, D Gavryushkin, G Jeschke, JP Cleveland, S Takahashi, P Szirmai, L Forró, E Emmanouilidou, R Singh, K Holczer*, Carbon, **188**, 393, (2022)
IF: 10.9, D1, No. of independent citations: 7
High concentration of negatively charged nitrogen-vacancy (NV⁻) centers was created in diamond single crystals containing approximately 100 ppm nitrogen using electron and neutron irradiation and subsequent thermal annealing in a stepwise manner. Continuous-wave electron paramagnetic resonance (EPR) was used to determine the transformation efficiency from isolated N atoms to NV⁻ centers in each production step and its highest value was as high as 17.5%. Charged vacancies are formed after electron irradiation as shown by EPR spectra, but the thermal annealing restores the sample quality as the defect signal diminishes. We find that about 25% of the vacancies form NVs during the annealing process. The large NV⁻ concentration allows observing orientation dependent spin-relaxation times and also determining the hyperfine and quadrupole coupling constants with high precision using electron spin echo (ESE) and electron-nuclear double resonance (ENDOR). We also observed the EPR signal associated with the so-called W16 centers, whose spectroscopic properties might imply a nitrogen dimer-vacancy center for its origin.
2. Optimization of Chromium-Doped Zinc Gallate Nanocrystals for Strong Near-Infrared Emission by Annealing *Mátyás M Rudolf, Gábor Bortel, Bence G Markus, Nikoletta Jegenyes, Vladimir Verkhovlyuk, Katalin Kamarás, Ferenc Simon, Adam Gali, David Beke*, ACS Applied Nano Materials, **5**, 8950, (2022)
IF: 6.14, D1, No. of independent citations: 7

Chromium-doped spinel crystals show long-lasting emissions in the near-infrared wavelength region. The emission can be activated by X-ray or ultraviolet–visible (UV–visible) light. Such properties make this material a promising candidate for background-free deep-tissue bioimaging, photodynamic or photon-induced therapy, and other applications. Here, we apply hydrothermal synthesis for the preparation of Cr-doped zinc gallate (ZnGa_2O_4) nanoparticles of small sizes with around 10 nm in diameter, which has the potential to be intravenously introduced to patients. We find that annealing of the as-prepared nanoparticles at 800 °C yields an order of magnitude increase in the emission intensity in the near-infrared wavelength region upon X-ray exposure with favorable long-lasting photoluminescence, which may be directly employed for deep-tissue cancer treatments when combined with IR700-mAb conjugate drug agents. We discuss the effect of annealing on the structural changes and the evolution of Cr defects of 10 nm Cr-doped zinc gallate nanoparticles by imaging techniques and monitoring their magneto-optical signals.

3. Enhancement of X-ray-Excited Red Luminescence of Chromium-Doped Zinc Gallate via Ultrasmall Silicon Carbide Nanocrystals *Dávid Beke, Marco V Nardi, Gábor Bortel, Melanie Timpel, Zolt Czigány, Luca Pasquali, Andrea Chiappini, Giorgio Bais, Mátyás Rudolf, Dóra Zalka, Franca Bigi, Francesca Rossi, László Bencs, Aron Pekker, Bence G Márkus, Giancarlo Salviati, Stephen E Sadow, Katalin Kamarás, Ferenc Simon, Adam Gali* Chemistry of Materials **33**, 2457, (2021)

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No. of independent citations: 9

X-ray-activated near-infrared luminescent nanoparticles are considered as new alternative optical probes due to being free of autofluorescence, while both their excitation and emission possess a high penetration efficacy in vivo. Herein, we report silicon carbide quantum dot sensitization of trivalent chromium-doped zinc gallate nanoparticles with enhanced near-infrared emission upon X-ray and UV–vis light excitation. We have found that a ZnGa_2O_4 shell is formed around the SiC nanoparticles during seeded hydrothermal growth, and SiC increases the emission efficiency up to 1 order of magnitude due to band alignment that channels the excited electrons to the chromium ion.

4. Room-Temperature Defect Qubits in Ultrasmall Nanocrystals *Dávid Beke, Jan Valenta, Gyula Károlyházy, Sándor Lenk, Zolt Czigány, Bence Gábor Márkus, Katalin Kamarás, Ferenc Simon, Adam Gali* The Journal of Physical Chemistry Letters **11**, 1675, (2020)

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No. of independent citations: 23

There is an urgent quest for room-temperature qubits in nanometer-sized, ultrasmall nanocrystals for quantum biosensing, hyperpolarization of biomolecules, and quantum information processing. Thus far, the preparation of such qubits at the nanoscale has remained futile. Here, we present a synthesis method that avoids any interaction of the solid with high-energy particles and uses self-propagated high-temperature synthesis with a subsequent electrochemical method, the no-photon exciton generation chemistry to produce room-temperature qubits in ultrasmall nanocrystals of sizes down to 3 nm with high yield. We first create the host silicon carbide (SiC) crystallites by high-temperature synthesis and then apply wet chemical etching, which results in ultrasmall SiC nanocrystals and facilitates the creation of thermally stable defect qubits in the material. We demonstrate room-temperature optically detected magnetic resonance signal of divacancy qubits with 3.5% contrast from these nanoparticles with emission wavelengths falling in the second biological window (1000–1380 nm). These results constitute the formation of nonperturbative bioagents for quantum sensing and efficient hyperpolarization.

5. Immunomodulatory potential of differently-terminated ultra-small silicon carbide nanoparticles *Tereza Bělinová, Iva Machová, David Beke, Anna Fučíková, Adam Gali, Zuzana Humlová, Jan Valenta, Marie Hubálek Kalbáčová*, Nanomaterials **10**, 573, (2020)

IF: 5.3, D1,

No. of independent citations: 4

Ultra-small nanoparticles with sizes comparable to those of pores in the cellular membrane possess significant potential for application in the field of biomedicine. Silicon carbide ultra-small nanoparticles with varying surface termination were tested for the biological system represented by different human cells (using a human osteoblastic cell line as the reference system and a monocyte/macrophage cell line as immune cells). The three tested nanoparticle surface terminations resulted in the observation of different effects on cell metabolic activity. These effects were mostly noticeable in cases of monocytic cells, where each type of particle caused a completely different response ('as-prepared' particles, i.e., were highly cytotoxic, –OH terminated particles slightly increased the metabolic activity, while –NH₂ terminated particles caused an almost doubled metabolic activity) after 24 h of incubation. Subsequently, the release of cytokines from such treated monocytes and their differentiation into activated cells was determined. The results revealed the potential modulation of immune cell behavior following stimulation with particular ultra-small nanoparticles, thus opening up new fields for novel silicon carbide nanoparticle biomedical applications.