



# załącznik do Regulaminu programu "visiting profesor"

Osoba zgłaszająca z PW	
Tytuł i stopień naukowy	Prof. dr hab. inż.
Imię i nazwisko	Agnieszka Adamczyk-Woźniak
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Propozycja osoby zgłasza	anej jako visiting professor				
Tytuł i stopień naukowy	Prof. Dr.				
Imię i nazwisko	Agnieszka Nowak-Król				
Dokładna afiliacja	Universität Würzburg, Institut für Anorganische Chemie and				
	Institute for Sustainable Chemistry & Catalysis with Boron, Am				
	Hubland, D-97074 Würzburg, Germany				
Mail kontaktowy	agnieszka.nowak-krol@uni-wuerzburg.de				
Opis osiągnięć	Agnieszka Nowak-Król graduated with honors from the Rzeszów University				
(1/2-1  strony)	of Technology in Poland, where she worked with Dr. Grażyna Groszek on				
	the synthesis of bioactive compounds. For her master's thesis, she was				
	awarded the distinction for Janina Janikowa Award of the Polish Chemical				
	Society for the best MSc thesis in chemistry in Poland in 2008. She earned				
	her doctorate at the Polish Academy of Sciences in Warsaw in 2013 with				
	Prof. Daniel Gryko. Her research focused on the design and synthesis of				
	porphyrinoids (porphyrins and corroles) with large two-photon absorption				
	cross-section and appropriate secondary properties, such as liquidity at room				
	temperature or liquid crystallinity. During her PhD thesis, she was the PI of				
	two grants, one funded by the Foundation for Polish Science (Ventures				
	Programme) and another one by the National Science Center. She then				
	continued her career as an Alexander von Humboldt Postdoctoral Fellow				
	Characteristic of the University of Währhung in Compared In the Währhung				
	Chemistry of the University of wurzburg in Germany. In the wurthner				
	group, she explored the chemistry and properties of perylene distinue dyes				
	and acceptor-donor-acceptor materials for organic electronics and				
	supramolecular dye architectures. In 2016, she started her independent				
	career as a group leader at the Center for Nanosystems Chemistry in				
	Würzburg In 2019 she received the prestigious Emmy-Noether grant				
	(€1.87 million) from the German Research Foundation to establish her				
	independent research group. In 2019, she received a call for a tenure-track				
	position from the University of Bonn, which she declined, and in 2020, she				
	accepted a tenure-track junior professor position at the Institute of Inorganic				
	Chemistry and the Institute for Sustainable Chemistry & Catalysis with				
	Boron of the University of Würzburg. She was promoted to professor in				
	2024. Agnieszka is the recipient of several awards and honors, including the				





Arnold Sommerfeld Prize of the Bavarian Academy of Sciences and Humanities, the Hector Research Career Development Award of the Hector Fellow Academy, the Thieme Chemistry Journals Award, the Bürgenstock JSP Fellowship of the Swiss Chemical Society, the Wojciech Swietoslawski Award, and the Zonta Award. She is a member of the Societas Humboldtiana Polonorum, Soltech, the Polish Chemical Society, and the German Chemical Society, and a member of the Early Career Advisory Board of *Organic Chemistry Frontiers*. Her research lies at the interface of organic, inorganic and materials chemistry. Her current activities focus on the development of helically chiral  $\pi$ -conjugated organoboron compounds, boron-containing polycyclic aromatic hydrocarbons, photoswitches, helicenes containing other main group elements and their applications in organic electronics and bioimaging.

Code of the	4606-VP-ES-000	15	Polish Barwniki Funkcjonalne v Współczesnej Chemii i T		Polish		we echnologii						
course						English			Functional Dyes in Modern Chemistry and Technology				
Type of the course	Specialty subject				_								
Course coordinator	Agnieszka Nowa	k-Król			Cour	purse teacher Agnieszka Nowak-Król							
Implementing unit	Faculty of Che	mistry	Scientif dise	ic discipli ciplines*	ne /	Chemistry, Materials Science, Chemical Engineering		ering					
Level of education	Doctoral S	chool	:	Semester		I		II	III 2025: on-site classes				
Language of the course	English												
Type of assessment	Assessment wi	th a grade	a grade Number of hours in a semester		rs in	60			ECTS credits		5		
Minimum number of participants	10		Maxi of	mum nun participan	nber its						Available for studer (BSc, MSc)	nts	<u>Yes</u> /No
Type of clas	ses	Lectu	ure	Aud cla	Auditory classes		Project classes		Laboratory		Seminar		
Number of hours	in a week	10	)			5		5			5		
	in a semester 30					15			15				

\* does not apply to the Researcher's Workshop

### 1. Prerequisites

Basic knowledge in chemistry and physics.

## 2. Course objectives

The course provides an overview of the characteristics of functional materials and their application in current chemistry and technology, e.g. organic electronics, photovoltaics, and bioimaging. The course will cover the new trends in the development of functional materials, recent achievements in selected applications and new directions. The challenges and benefits of the use of chiral materials will be discussed in more detail. The students will become acquainted with the fundamental principles that underpin the operation of devices, the characterization of functional chiral and achiral materials, the critical parameters, and the structure-property





relationships. This knowledge will enable the assessment of the suitability of a material for a given application and the critical evaluation of published data.

Emphasis will also be placed on communication skills. The aim is to prepare the graduates for active participation in conferences and seminars in various roles. To this end, students will give a short talk on a given topic (physical phenomenon, device, compound class), introduce the speaker, manage questions and answers, and participate in a scientific discussion.

3. Course content (separate for each type of classes)
Lecture

Functional materials: historical background, selected classes of  $\pi$ -conjugated compounds, characterization and properties, tuning of optical and electronic properties of polycyclic aromatic hydrocarbons, thermally-activated delayed fluorescence, narrowband emission, room-temperature phosphorescence, two-photon absorption, application of functional materials (e.g. solar cells, transistors, organic light-emitting diodes, bioimaging), chirality and historical background, types of chiral compounds, symmetry and point groups, properties of chiral materials (optical rotation, circular dichroism, circularly polarized light, chiral-induced spin selectivity, magnetochiral anisotropy), figures of merit, configurational stability, molecular geometry and the packing arrangement in the solid state, determination of an enantiomerization/distereomerization barrier, topology, selected synthetic approaches to chiral compounds, boron-containing helicenes and other boron-containing chiral compounds, application of chiral materials (e.g. in solar cells, transistor devices, circularly polarized organic light-emitting diodes, polarization-selective photodetectors, spintronic devices).

## Seminar

Discussion and extended analysis of the topics covered in the lecture, e.g. device operation, photophysical properties, point group determination, assigning the absolute configuration of chiral compounds, determination of enantiomerization barriers (choice of the method, Eyring equation), calculation of the dissymmetry factors based on electric and magnetic transition dipole moments, CPL brightness based on experimental data, solvatochromism, reorganization energy.

### Project classes

Presentations on selected topics, i.e. either a physical phenomenon or a compound class or a device type based on several selected publications, comparing and critically evaluating the published work. Another course participant will introduce the speaker and manage questions. All participants are expected to participate in the discussion.

4. Learning outcomes					
Type of learning outcomes	Learning outcomes description	Reference to the learning outcomes of the WUT DS	Learning outcomes verification methods*		
	Knowledge – the gra	aduate			
K01	is familiar with different photophysical, electronic and chiroptical properties of functional materials	SD_W2, SD_W3	active participation during classes; test		
K02	understands the structure-property relationships	SD_W2, SD_W3	active participation during classes; test		
K03	is familiar with different areas of application of functional dyes	SD_W1, SD_W2, SD_W3, SD_W4, SD_W5	active participation during classes; test		
K04	is familiar with different methods to determine the enantiomerization/distereomerization barrier	SD_W2, SD_W3	active participation during classes; test		





K05	is familiar with selected synthetic approaches to chiral compounds, in particular boron- containing helicenes	SD_W2, SD_W3	active participation during classes; test
K06	understands the concept of topology in chemistry	SD_W2, SD_W3	active participation during classes; test
K07	understands the fundamental principles that underpin the operation of devices	SD_W1, SD_W2, SD_W3, SD_W4, SD_W5	active participation during classes; test, presentation evaluation
	Skills – the graduat	e can	
S01	correlate the properties of functional materials with their electronic structures and packing arrangements	SD_U1, SD_U2	active participation during classes; tests, presentation evaluation
S02	determine the point group and assign the absolute configuration of a chiral compound	SD_U1	active participation during classes; tests
S03	assess the configurational stability of a chiral material and select a method to determine the enantiomerization/distereomerization barrier	SD_U1, SD_U2, SD_U7	active participation during classes; tests
S04	evaluate the properties of compounds and materials for a given application	SD_U2, SD_U3	active participation during classes; tests, presentation evaluation
S05	critically assess the device operation	SD_U2	active participation during classes; tests
S06	use English at a B2+ level to effectively communicate during the classes and presentations	SD_U6	presentation evaluation, presentation evaluation
S07	can communicate scientific content in a clear and accessible way	SD_U4, SD_U6	presentation evaluation
S08	can chair a scientific lecture and participate in a scientific discussion	SD_U5, SD_U6	active participation during classes
S09	can work in a group on a given project, topic	SD_U8	active participation during classes
	Social competences – the	e graduate	
SC01	can critically evaluate the achievements within a scientific discipline and situate given scientific work in a broader context	SD_K1	presentation evaluation
SC02	critically evaluate scientific publications	SD_K1, SD_K5	presentation evaluation, active participation during classes

\*Allowed learning outcomes verification methods: exam; oral exam; oral test; project evaluation; report evaluation; presentation evaluation; active participation during classes; homework; tests

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Results of a test + evaluation of a presentation + activity





## 6. Literature

Materials from the lecture

M. Rickhaus, L. Jundt, M. Mayor, Determining Inversion Barriers in Atropisomers – A Tutorial for Organic Chemists. *Chimia* **2016**, *70*, 192–202.

K. Kato, Y. Segawa, K. Itami, Symmetric Multiple Carbohelicenes. Synlett 2019, 30, 370-377.

A. Nowak-Król, P. T. Geppert, K. R. Naveen, Boron-containing helicenes as new generation of chiral materials: opportunities and challenges of leaving the flatland. *Chem. Sci.* **2024**, *15*, 7408-7440.

J. R. Brandt, F. Salerno, M. J. Fuchter. The added value of small-molecule chirality in technological applications. *Nat. Rev. Chem.* **2017**, *1*, 0045.

F. Furlan, J. M. Moreno-Naranjo, N. Gasparini, S. Feldmann, J. Wade, M. J. Fuchter. Chiral materials and mechanisms for circularly polarized light-emitting diodes. *Nat. Photonics* **2024**, *18*, 658–668.

M. D. Ward, J. Wade, X. Shi, J. Nelson, A. J. Campbell, M. J. Fuchter. Highly Selective High-Speed Circularly Polarized Photodiodes Based on  $\pi$ -Conjugated Polymers. *Adv. Opt. Mater.* **2022**, *10*, 2101044.

V. Kiran, S. P. Mathew, S. R. Cohen, I. Hernández Delgado, J. Lacour, R. Naaman, Helicenes – A New Class of Organic Spin Filter. *Adv. Mater.* **2016**, *28*, 1957–1962.

J. Wade, F. Salerno, R. C. Kilbride, D. K. Kim, J. A. Schmidt, J. A. Smith, L. M. LeBlanc, E. H. Wolpert, A. A. Adeleke, E. R. Johnson, J. Nelson, T. Mori, K. E. Jelfs, S. Heutz, M. J. Fuchter. Controlling anisotropic properties by manipulating the orientation of chiral small molecules. *Nat. Chem.* **2022**, *14*, 1383–1389.

J. L. Greenfield, J. Wade, J. R. Brandt, X. Shi, T. J. Penfold, M. J. Fuchter. Pathways to increase the dissymmetry in the interaction of chiral light and chiral molecules. *Chem. Sci.* **2021**, *12*, 8589–8602.

J. Crassous, M. J. Fuchter, D. E. Freedman, N. A. Kotov, J. Moon, M. C. Beard, S. Feldmann. Materials for chiral light control. *Nat. Rev. Mater.* **2023**, *8*, 365–371.

L. Frédéric, A. Desmarchelier, L. Favereau, G. Pieters. Designs and Applications of Circularly Polarized Thermally Activated Delayed Fluorescence Molecules. *Adv. Funct. Mater.* **2021**, *31*, 2010281.

P. C. Mondal, C. Fontanesi, D. H. Waldeck, R. Naaman, Spin-Dependent Transport through Chiral Molecules Studied by Spin-Dependent Electrochemistry. *Acc. Chem. Res.* **2016**, *49*, 2560–2568.

Ray, K.; Ananthavel, S. P.; Waldeck, D. H.; Naaman, R. Asymmetric Scattering of Polarized Electrons by Organized Organic Films of Chiral Molecules. *Science* **1999**, *283*, 814–816.

https://www.nature.com/scitable/ebooks/english-communication-for-scientists-14053993/contents/

Further reading will be provided during the lecture.

7. PhD student's workload necessary to achieve the learning outcomes**						
No.	Description	Number of hours				
1	Hours of scheduled instruction given by the academic teacher in the classroom	60				
2	2 Hours of consultations with the academic teacher, exams, tests, etc. 15					
3	Amount of time devoted to the preparation for classes, preparation of presentations, reports, projects, homework	45				
4	4 Amount of time devoted to the preparation for exams, test, assessments 10					
	Total number of hours 130					
	ECTS credits 5					
** 1 ECTS = 25-30 hours of the PhD students work (2 ECTS = 60 hours: 4 ECTS = 110 hours, etc.)						

\*\* 1 ECTS = 25-30 hours of the PhD students work (2 ECTS = 60 hours; 4 ECTS = 110 hours, etc.)

8. Additional information	
Number of ECTS credits for classes requiring direct participation of academic teachers	





Number of ECTS credits earned by a student in a practical course