

Name of the advisor: Julien Guthmuller**Academic title:** associate professorOrcid ID number: <https://orcid.org/0000-0002-9877-6290>**Department of** Theoretical Physics and Quantum Information**Faculty of** Applied Physics and Mathematics**Gdańsk University of Technology****Phone:** +48 58 347 28 89**E-mail:** julien.guthmuller@pg.edu.pl**Personal web page:** www.pg.edu.pl/katedra-fizyki-teoretycznej-i-informatyki-kwantowej**Disciplineⁱ** physical sciences, chemical sciences**Bibliometric indicators**

1.	Number of journal publications in WoS/ Scopus	54/53
2.	Citations (WoS/Scopus) excluding self-citations	927 /963
3.	Hirsch index (WoS/Scopus)	22 /22
4.	Hirsch index in Google Scholar	24
5.	Citations in Google Scholar	1404

1. The number of PhD students who have graduated under your supervision: 0

2. The number of PhD students currently supervised: 2

3. Are you currently accepting new PhD students:

a. Polish Yes

b. Foreign Yes

Research interests or topics offered for PhD research (no more than 2000 characters)ⁱⁱ

The research interests concern the development and application of quantum chemistry methods for the understanding and prediction of molecular properties and spectra (e.g. structural, electronic and optical properties). In particular, the investigations focus on the spectroscopies of absorption, emission, photoelectron and resonance Raman as well as on the process of photo-induced electron transfer. The applications concern organic and inorganic compounds for solar energy conversion and molecular sensors. These systems can be used e.g. in dye-sensitized solar cells or as supramolecular photocatalysts for the generation of molecular hydrogen. In this frame, theoretical calculations provide predictions and interpretations of the optical and electronic properties, helping in the design of new and more efficient systems.

PhD Advisor form

Funding or special equipment needed to carry out a PhD project ⁱⁱⁱ:

1. Is funding available for experimental work: Not applicable
2. Is the equipment needed to complete a PhD project available in your lab/department: Yes

Most recent publications in WoS/SCOPUS journal – no more than 5 published after 1.01.2017

No	Authors/title/journal	Journal IF/Quartile – for WoS and SNIP/ CiteScore for SCOPUS	Publication year
1.	M. Martynow, S. Kupfer, S. Rau, and J. Guthmuller, Excited state properties of a series of molecular photocatalysts investigated by time dependent density functional theory, Phys. Chem. Chem. Phys. DOI: 10.1039/c9cp00335e	IF: 3.906 Quartile: Q1 SNIP: 1.089 CiteScore: 4.04	2019
2.	M. Staniszewska, S. Kupfer, and J. Guthmuller, Theoretical investigation of the electron-transfer dynamics and photodegradation pathways in a hydrogen-evolving ruthenium-palladium photocatalyst, Chem. Eur. J. 24, 11166-11176.	IF: 5.160 Quartile: Q1 SNIP: 1.020 CiteScore: 4.97	2018
3.	J. Guthmuller, The role of Herzberg-Teller effects on the resonance Raman spectrum of trans-porphycene investigated by time dependent density functional theory, J. Chem. Phys. 148, 124107.	IF: 2.843 Quartile: Q2 SNIP: 0.926 CiteScore: 2.50	2018
4.	M. Staniszewska, S. Kupfer, M. Łabuda, and J. Guthmuller, Theoretical Assessment of Excited State Gradients and Resonance Raman Intensities for the Azobenzene Molecule, J. Chem. Theory Comput. 13, 1263-1274.	IF: 5.399 Quartile: Q1 SNIP: 1.476 CiteScore: 5.25	2017
5.	M. A. Śmiałek, J. Guthmuller, M. A. MacDonald, L. Zuin, J. Delwiche, M. J. Hubin-Franskin, T. Leśniewski, N. J. Mason, and P. Limão-Vieira, Photoelectron spectroscopy of a series of acetate and propionate esters, J. Quan. Spect. Rad. Trans. 200, 206-214.	IF: 2.600 Quartile: Q2 SNIP: 1.320 CiteScore: 2.44	2017

Most recent externally funded projects you were involved in – no more than 3

No	Project title, the name of the Princ. Investigator (PI) and the institution the project was carried out	Year awarded	Role in the project
1.	Horizon 2020 Marie Skłodowska-Curie Innovative Training Networks project "Molecular logic lab-on-a-vesicle for intracellular diagnostics – LOGIC LAB" financed by the European Commission. Project PI: Prof. Benjamin Dietzek (Jena), GUT Party coordinator: dr hab. Julien Guthmuller	2018	co-PI
2.	NCN HARMONIA 6 project "Theoretical and spectroscopic investigation of the photochemistry of supramolecular photocatalysts for hydrogen generation" financed by the Narodowe Centrum Nauki. Project PI: dr hab. Julien Guthmuller (GUT).	2015	PI

PhD Advisor form

3.	Marie Curie Career Integration Grant, Project VIBRAMAN “Theoretical simulation of vibrational spectroscopies based on the Raman effect” financed by the 7th Framework Programme of the European Union. Project PI: Prof. Józef Sienkiewicz (GUT).	2012	R
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Additional relevant information – (no more than 1600 charters)^{iv}

ⁱ You may select up to two disciplines out of 12 disciplines represented in the Doctoral School

ⁱⁱ Observe the limit of not more than 300 words

ⁱⁱⁱ Leave only one answer

^{iv} Add any other relevant information eg. awards for PHD students whom you supervised (no more than 200 words)