Prospective supervisor's form

Name of the supervisor: JULIEN GUTHMULLER

Academic title: PhD.Sc.

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Faculty of Applied Physics and Mathematics

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Discipline[i] physical sciences [NF] chemical sciences [NCh]

Optional

Key words (obligatory four key words describing research interests / expertise):

Quantum chemistry

Electron transfer

Optical properties of molecules

Resonance Raman spectra

Bibliometric indicators

1. Number of journal publications in WoS/ Scopus 57/57
2. Citations excluding self-citations WoS 1032 Scopus 1051
3. Hirsch index WoS 23 Scopus 23

1. The number of PhD students who have graduated under your supervision: 0
2. The number of PhD students currently supervised:
   a. within the current doctoral school 0
   b. within doctoral studies (previous system) 3
3. Are you currently accepting new PhD students:
   a. Polish *Yes/No* Yes
   b. Foreign *Yes/No* Yes

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

The general 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 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. 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 topic:
To satisfy the energy demand of modern society it is vital to provide new sources of energy. A promising source of regenerative energy is sunlight. Different attempts of utilizing solar energy are being pursued, ranging from artificial photosynthesis to direct generation of electricity from solar cells. In this respect, the aim of the PhD topic is to design light-harvesting compounds and supramolecular catalysts based on a fully theoretical approach. Therefore, the PhD student will employ and develop theoretical methods to find novel molecular photosensitizers and photocatalysts with desired properties and functions. In particular, these systems should (i) absorb light in the entire visible region and the near IR, (ii) store and transfer efficiently multi-electrons to an acceptor site, (iii) reduce charge recombination processes, and (iv) be composed of environmentally friendly and earth-abundant elements (e.g., iron). The studies will be conducted applying state-of-the-art quantum chemical calculations, such as multiconfigurational methods and TDDFT.
The research project will be realized in close cooperation with our German partner Dr. Stephan Kupfer (Jena).

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

1. Is funding available for experimental work: *Yes/No/not needed* — not needed
2. Is the equipment needed to complete a PhD project available in your lab/department: *Yes/No/not needed* — Yes

Most important publications – no more than 5 published after 1.01.2018

No	Authors/title/journal	Number of points according to the current list of the Ministry of Science and Higher Education	Publication year
1.	M. Martynow, D. Głowienka, J. Szmytkowski, Y. Galagan, and J. Guthmuller, ChemPhysChem 20 (2019) 3228-3237, Influence of Orientational Disorder on the Optical Absorption Properties of the Hybrid Metal-Halide Perovskite CH3NH3PbI3. A Combined DFT/TD-DFT and Experimental Study.	100	2019
2.	M. Staniszewska, S. Kupfer, and J. Guthmuller, J. Phys. Chem. C 123 (2019) 16003-16013, Effect of the Catalytic Center on the Electron Transfer Dynamics in Hydrogen-Evolving Ruthenium-Based Photocatalysts Investigated by Theoretical Calculations.	140	2019

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3.	M. Martynow, S. Kupfer, S. Rau, and J. Guthmuller, Phys. Chem. Chem. Phys. 21 (2019) 9052-9060, Excited state properties of a series of molecular photocatalysts investigated by time dependent density functional theory.	100	2019
4.	M. Staniszewska, S. Kupfer, and J. Guthmuller, Chem. Eur. J. 24 (2018) 11166-11176, Theoretical investigation of the electron-transfer dynamics and photodegradation pathways in a hydrogen-evolving ruthenium-palladium photocatalyst.	140	2018
5.	J. Guthmuller, J. Chem. Phys. 148 (2018) 124107, The role of Herzberg-Teller effects on the resonance Raman spectrum of trans-porphycene investigated by time dependent density functional theory.	100	2018

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

No	Project title, the name of the Principal Investigator (PI) and the institution the project was carried out	Years	Role in the project [iv]
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	2018-2022	Co-I
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).	2015-2018	PI
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).	2012-2016	R

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Additional relevant information – (no more than 1600 characters)[v]

[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 2000 characters

[iii] Leave only one answer

[iv] Select the role in the project: PI stands for principal investigator (refers to the holder of an independent grant and the lead researcher for the grant project), Co-I for co-investigator (Co-I assists the principal investigator in the management and leadership of the research project), R for researcher

[v] Add any other relevant information e.g. awards for PhD students whom you supervised (no more than 1600 characters)