

# Prospective supervisor's form

Name of the supervisor: Jacek Czub

Academic title: PhD.Sc.Eng.

Orcid ID number: <https://orcid.org/0000-https://orcid.org/0000-0003-3639-6935>

Gdańsk University of Technology Faculty of Chemistry

Department of Physical Chemistry

Phone: +48 535970599

E-mail: jacek.czub@pg.edu.pl

Personal web page: <https://pg.edu.pl/kbm>

Discipline: chemical sciences [NCh] none

Optional

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

# molecular biophysics

# theoretical and computational chemistr

# molecular dynamics

# statistical thermodynamics

## Bibliometric indicators

1. Number of journal publications in WoS/ Scopus 44/44

2. Citations excluding self-citations WoS 712 Scopus 690

3. Hirsch index WoS 17 Scopus 17

1. The number of PhD students who have graduated under your supervision: 3

2. The number of PhD students currently supervised:

a. within the current doctoral school 2

b. within doctoral studies (previous syst 4

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)<sup>ii</sup>

We are a dynamically developing team of researchers investigating the molecular mechanisms and driving forces behind biologically relevant phenomena. In our research we employ numerical simulations based on molecular models, as well as combine multidisciplinary knowledge from the fields of chemistry, physics, biology and computer science. In scientific work, we actively encourage a creative and inquisitive atmosphere by fostering open exchange of thoughts, ideas and expertise.

In particular, our research, based on:

- i) numerical simulations of classical and quantum chemical (ab initio) molecular dynamics
- ii) calculation and decomposition of free energies of molecular interactions rooted in statistical mechanics,
- iii) analysis of numerical data (data science)

is focused on the issues of:

- i) conformational changes and energy transmission within proteins,
- ii) specificity in protein-ligand, protein-DNA and protein-protein interactions, also for applications in knowledge-based drug design,
- iii) impact of the lipid bilayer environment on the conformations, orientation, transport and interactions of biologically relevant molecules.

For more specific information about possible topics of PhD research, please, visit our webpage at [www.chem.pg.edu.pl/kbm](http://www.chem.pg.edu.pl/kbm) and/or contact the PI directly ([jacek.czub@pg.edu.pl](mailto:jacek.czub@pg.edu.pl)).

### Funding or special equipment needed to carry out a PhD project <sup>iii</sup>:

1. Is funding available for experimental work: *Yes/No/not needed*

2. Is the equipment needed to complete a PhD project available in your lab/department: *Yes/No/not needed*

### 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.	B. Adamczak, M. Kogut, J. Czub. Effect of osmolytes on the thermal stability of proteins: replica exchange simulations of Trp-cage in urea and betaine solutions. <i>Phys. Chem. Chem. Phys.</i>	100	2018
2.	E. Grela, M. Wieczór, (...), J. Czub, W. Gruszecki. Mechanism of Binding of an Antifungal Antibiotic Amphotericin B to Lipid Membranes: An Insight from Combined Single Membrane Imaging, Micro-Spectroscopy, and Molecular Dynamics. <i>Mol. Pharmaceut.</i>	140	2018

### Prospective supervisor's form

3.	M. Kogut, C. Kleist, J. Czub Molecular dynamics simulations reveal the balance of forces governing the formation of a guanine tetrad – a common structural unit of G-quadruplex DNA. PLoS Comput. Biol.	140	2019
4.	M. Wieczor, J. Czub Telomere uncapping by common oxidative guanine lesions: Insights from atomistic models. Free Rad. Bio. Med	140	2020
5.	B. Tomiczek, W. Delewski, L. Nierzwicki, M. Stolarska, I. Grochowina, B. Schilke, R. Dutkiewicz <sup>1</sup> , M.A. Uzarska, S.J. Ciesielski, J. Czub, E.A. Craig, J. Marszalek Two-step mechanism of J-domain action in driving Hsp70 function, PLoS Comput. Biol.	140	2020

#### 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 <sup>iv</sup>
1.	"Telomeres as targets for anticancer drug development – a computational approach", funding agency: Foundation for Polish Science, institution: Gdansk University of Technology	2012-2015	PI
2.	"Molecular mechanism of energy transfer and conversion in catalytic portion of ATP synthase", funding agency: Ministry of Science and Higher Education (PL), institution: Gdansk University of Technology	2013-2016	PI
3.	"Molecular picture of the mechanochemical coupling in ATP synthase as a conceptual framework for the development of novel antimicrobial drugs", funding agency: National Science Centre (PL), institution: Gdansk University of Technology	2018-2023	PI

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### Additional relevant information – (no more than 1600 characters)<sup>v</sup>

Your profile: i) candidates have to hold a MSc degree and be eligible to enroll in a PhD program at GUT, ii) strong background in physics, physical chemistry, applied mathematics, computer science or related fields and commitment to pursue theoretical and numerical research on real-life problems, iii) experience in applying computational tools to study biological or chemical phenomena will be an advantage, iv) programming experience (python, C/C++, etc.) is not required but would be beneficial, v) fluency in English.

What we offer: i) PhD scholarships on top of the standard salary, ii) opportunities to publish research findings in high-impact scientific journals (e.g. J.Am.Chem.Sci, Nucleic Acids Res., J.Phys.Chem.Lett., etc, see full list of papers at [www.chem.pg.edu.pl/kbm/publications](http://www.chem.pg.edu.pl/kbm/publications)) iii) opportunities to pursue scientific internships in the renowned Max Planck Institute for Biophysical Chemistry in Goettingen, as well as at the Leiden University (Netherlands), iv) successful preparation for postdoctoral training at renowned research institutions (so far, e.g., IRB Barcelona, University of California Riverside, University of Gdansk, also within Marie Curie Post-doctoral Fellowships)

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

<sup>ii</sup> Observe the limit of not more than 2000 characters

<sup>iii</sup> Leave only one answer

<sup>iv</sup> 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

<sup>v</sup> Add any other relevant information e.g. awards for PhD students whom you supervised (no more than 1600 characters)