PhD Advisor form

Name of the advisor: Jacek Czub

Academic title: Ph.D, D.Sc., Eng.

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Discipline[i] chemical sciences, physical sciences

Bibliometric indicators

1.	Number of journal publications in WoS/ Scopus	41 (WoS)/41 (Scopus)
2.	Citations (WoS/Scopus) excluding self-citations	627 (WoS)/ 617 (Scopus)
3.	Hirsch index (WoS/Scopus)	16 (WoS)/ 16 (Scopus)
4.	Hirsch index in Google Scholar	17
5.	Citations in Google Scholar	980

1. The number of PhD students who have graduated under your supervision: 0
2. The number of PhD students currently supervised: 7
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]

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 and/or contact the PI directly (jacek.czub@pg.edu.pl).

PhD Advisor form

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

1. Is funding available for experimental work: Yes
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.	J. Czub, M. Wieczór, B. Prokopowicz, H. Grubmüller. Mechanochemical Energy Transduction during the Main Rotary Step in the Synthesis Cycle of F1-ATPase. J. Am. Chem. Soc.	14.357/Q1 (WoS) 14.05/2.641 (Scopus)	2017
2.	M. Wieczór, J. Czub. How proteins bind to DNA: target discrimination and dynamic sequence search by the telomeric protein TRF1. Nucleic Acids Res.	11.561/Q1 (WoS) 10.84/3.028 (Scopus)	2017
3.	P. Wityk, M. Wieczór, S. Makurat, L. Chomicz-Mańka, J. Czub, J. Rak. Dominant pathways of adenosyl radical-induced DNA damage revealed by QM/MM metadynamics. J. Chem. Theory Comput.	5.399/Q1 (WoS) 5.25/1.476 (Scopus)	2017
4.	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. Phys. Chem. Chem. Phys.	3.906/Q1 (WoS) 4.04/1.089 (Scopus)	2018
5.	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. Mol. Pharmaceut.	4.556/Q1 (Wos) 4.86/1.24 (Scopus)	2018

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.	"Telomeres as targets for anticancer drug development – a computational approach", funding agency: Foundation for Polish Science, institution: Gdansk University of Technology	2012	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	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 Universtiy of Technology	2018	PI

Additional relevant information – (no more than 1600 charters)[iv]

One PhD position to study the mechanisms of action and inhibition of ATP synthase by means of molecular simulations is currently available. 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.), v) fluency in English. What we offer: i) PhD scholarship of 2500 z³/month (tax-exempt, in addition to the standard PhD scholarship in Poland), paid for full 4 years, starting on October 1, 2019; when adjusted for the costs of living in Gdansk, the total salary is competitive while benefits include health insurance in Poland and EU, ii) the project provides opportunities to pursue scientific internships in the renowned Max Planck Institute for Biophysical Chemistry in Goettingen, as well as at the Leiden University (Netherlands). Job description: preparing, performing and analyzing molecular dynamics simulations aimed at understanding the mechanism of action of ATP synthase, with a special emphasis on the differences between mammalian and microbial forms of the enzyme. Studies on the effect of Fo-ATPase inhibitors on the mechanism of proton translocation using free energy simulations and QM/MM ab-initio molecular dynamics.

[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)