Prospective supervisor's form

Name of the supervisor: Maciej Śmiechowski

Academic title: PhD. DSc. Eng.

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Faculty of Chemistry

Gdańsk University of Technology **Department of** Physical Chemistry

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Discipline[i] chemical sciences [NCh] none

Optional

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

physical chemistry

computational chemistry

molecular dynamics

solution chemistry

Bibliometric indicators

1. Number of journal publications in WoS/ Scopus 31 / 32
2. Citations excluding self-citations WoS 422 Scopus 437
3. Hirsch index WoS 14 Scopus 15

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 0
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 current research concerns the application of computational chemistry in solution chemistry. The prospective Ph.D. student can partake in several projects from the area of computational solution chemistry in close cooperation with experimental teams, thus offering the chance for research work in an interdisciplinary environment.
1. Water is a unique solvent as a natural environment of all cellular life. We study hydration of electrolytes and small models of biomolecules, and the proposed research concerns the application of computational chemistry in unraveling the structure and dynamics of hydrated compounds at a molecular level, complementing the experimental data obtained by infrared spectroscopy and other techniques.
2. Water is also an interesting solvent that is able to accommodate hydrophobic parts of biomolecules. This phenomenon, known as hydrophobic hydration, is studied by us on small-scale models, leading to better understanding of this biochemically relevant mechanism on an atomistic scale.
3. Non-aqueous solvents are particularly important whenever water is an unwanted component in the technological process, e.g., in electrochemistry. We study the structure and dynamics of molecular solvents' mixtures, paying close attention to the nature of interactions between components. The emerging science of deep eutectic solvents is a particularly perspective area of potential research.
All these topics are actively pursued at present as evidenced by the publications' list below. The prospective Ph.D. student is expected to be willing to engage in computational chemistry studies and a strong background in physical and/or theoretical chemistry is beneficial. The techniques used in the proposed topics include:
1. molecular dynamics simulations on a large scale, particularly with modern polarizable force fields
2. ab initio molecular dynamics using density functional theory at a smaller scale
3. quantum mechanical calculations for accurate thermodynamics

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.	B. Nowosielski, M. Jamrógiewicz, J. Łuczak, M. Śmiechowski, D. Warmińska, "Experimental and predicted physicochemical properties of monopropanolamine-based deep eutectic solvents", J. Mol. Liquids 309 (2020) 113110	100	2020
2.	D. Warmińska, M. Śmiechowski, "Thermophysical study of the binary mixtures of triethyl phosphate with N-methylformamide, N,N-dimethylformamide and N,N-dimethylacetamide – Experimental and theoretical approach", J. Mol. Liquids 304 (2020) 112778	100	2020

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3.	A. Panuszko, P. Bruździak, M. Śmiechowski, M. Stasiulewicz, J. Stefaniak, J. Stangret, "DMSO hydration redefined: Unraveling the hydrophobic hydration of solutes with a mixed hydrophilic–hydrophobic characteristic", J. Mol. Liquids 294 (2019) 111661	100	2019
4.	M. Leśniewski, M. Śmiechowski, "Communication: Inside the water wheel: Intrinsic differences between hydrated tetraphenylphosphonium and tetraphenylborate ions", J. Chem. Phys. 149 (2018) 171101	100	2018
5.	M. Śmiechowski, "Unusual Influence of Fluorinated Anions on the Stretching Vibrations of Liquid Water", J. Phys. Chem. B 122 (2018) 3141–3152	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.	National Science Center (NCN) grant no. 2013/11/B/NZ1/02258, "Protein stability in aqueous solutions of osmolytes studied through complementary theoretical and experimental approach", PI Prof. Dr. Janusz Stangret, Gdańsk University of Technology	2014–2017	R
2.	Deutsche Forschungsgemeinschaft grant no. 193464650, "Theoretical vibrational spectroscopy of aqueous solutions", PI Prof. Dr. Dominik Marx, Ruhr-Universität Bochum	2011–2013	R
3.	Ministry of Science and Higher Education grant no. N N204 3799 33, "Characteristics of hydration layers of selected electrolytes and non-electrolytes as models for the hydration of biomolecules", PI Prof. Dr. Janusz Stangret, Gdańsk University of Technology	2007–2010	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)