CeNT-36-2024

Director of Centre of New Technologies of the University of Warsaw, with the Project Leader, announce opening of the competition for the position of PhD Student in the Chemical and Biological Systems Simulation Laboratory – Centre of New Technologies of the University of Warsaw.

JOB OFFER

Position in the project:	PhD Student
Laboratory:	Chemical and Biological Systems Simulation Laboratory
Scientific discipline:	Chemical sciences
Keywords:	Computational modelling, quantum chemistry, organiometallic chemistry
Job type (employment contract/stipend):	Stipend
Part-time/full-time:	Part-time
Number of job offers:	1
Remuneration/stipend amount/month:	3000 – 4000 PLN gross gross
Position starts on:	between 01.01.2025 and 01.02.2025
Maximum period of contract/stipend agreement:	9 months with the possibility of extension up to 18 months
Institution:	Centre of New Technologies, University of Warsaw
Project leader:	Professor Bartosz Trzaskowski
Project title:	Bis-carbene ruthenium complexes as specialized olefin metathesis catalysts
NCN programme:	NCN OPUS 22
Project description:	The main goal of this research project is a systematic study of new bis-N-heterocyclic carbene (bis-NHC) and other bis-carbene ruthenium complexes as olefin metathesis catalysts for reactions, which are difficult to perform using standard ruthenium metathesis catalysts. The main part of this project consists of the design and computational modelling of ruthenium complexes incorporating not one carbene (as in standard metathesis catalysts), but two carbenes and their potential use in demanding olefin metathesis reactions such as ring opening metathesis polymerization (ROMP) and selective ring closing metathesis (RCM) to yield tetrasubstituted double bonds. In this work, we will use a quantum chemistry approach to a) obtain a better understanding of the structural and electronic features of ruthenium complexes and carbenes that allow the formation of such bis-NHC systems in contrast to systems containing a single NHC moiety, b) explore the vast chemical space of potential bis-NHC ruthenium complexes with respect to their stability, c) study the entire catalytic pathways of selected olefin metathesis reactions

	catalyzed by bis-carbene ruthenium complexes to test their applicability to perform such reactions, and d) synthesize selected bis-NHC and bis-carbene complexes to validate out computational results.
Key responsibilities include:	- design and modelling of new carbenes and transition metal complexes as well as their reaction paths - analysis of the obtained data - active participation in lab meetings, scientific seminars and international conferences - participation in the data preparation and writing of manuscripts
Profile of candidates/requirements:	The competition is open for persons who meet the conditions specified in the regulations on the allocation of resources for the implementation of tasks financed by the National Science Centre for OPUS 22 grant. MSc degree in chemistry or related discipline. The MSc degree should be obtained before the date of employment in the project. - Confirmed status of a PhD student (on the date of starting work in the project at the latest). - very good knowledge of mechanism of organic reactions - very good knowledge and experience in computational quantum chemistry methods used to describe small organic / organometallic / catalytic systems - very good command of English - scientific achievements documented by publications in recognized journals - strong analytical and problem-solving skills as well as excellent communication skills
Required documents:	1. Cover letter 2. Current curriculum vitae 3. Copy of MSc certificate (or, if the MSc certificate has not been obtained yet, a certificate/document about the date of MSc defense); 4. Document confirming the status of PhD Student (to be provided before starting work in the project); 5. Signed information on the personal data processing. Before entering the competition, candidates are obliged to familiarise themselves with Internal Reporting Procedure.
We offer:	- an opportunity to participate in a multidisciplinary project in one of the best scientific institutions in Poland - stimulating, young and friendly work environment - access to state-of-art equipment - opportunities for interdisciplinary and international collaborations

Please submit the following documents to:	b.trzaskowski@cent.uw.edu.pl with the title PhD application
Application deadline:	30.11.2024
Date of announcing the results:	05.12.2024
Method of notification about the results:	E-mail, CeNT website