JOB OFFER

Position in the project:	PhD Student
Scientific discipline:	chemistry
Job type (employment contract/stipend):	Scholarship
Number of job offers:	1
Remuneration/stipend amount/month (*"X0 000 PLN of full remuneration cost, i.e. expected net salary at X 000 PLN"*):	3500
Position starts on:	01.09.2019
Maximum period of contract/stipend agreement:	3 years
Institution:	Centre of New Technologies, University of Warsaw
Project leader:	dr hab. Bartosz Trzaskowski
Project title:	Catenanes as new tools for stereoselective catalysts
Project description:	The main goal of this research project is a systematic study of homogenous catalysts based on mechanically interlocked molecules directed toward better understanding of the fundamental aspects of their action. The main part of this project consists of the design and computational modelling of new mechanically interlocked catalysts incorporating carbenes in their structure. We will focus on the use of such systems in both organocatalysis as well as transition metal catalysis, with particular emphasis on designing candidates for efficient stereoselective metathesis catalysts. Controlling stereoselectivity in metathesis reactions, and cross-metathesis in particular, has long been a goal of research, as there is a pressing need to develop reliable routes to stereopure internal olefin products. In this work we will use a combined molecular dynamics / reactive force-field / quantum chemistry approach to explore both the static and dynamic properties of the newly designed systems.
Key responsibilities include:	1. Design and modelling of electronic properties of mechanically interlocked molecules 2. Analysis of the obtained data 3. Active participation in lab meetings, scientific seminars and international conferences. 4. Participation in the data preparation and writing of manuscripts.
Profile of candidates/requirements:	1. Current PhD student in chemistry, physics or related fields of Polish university (or about to become a PhD student by the end of October 2019) 2. MSc degree (or equivalent) in chemistry, physics or related fields (or about to graduate until end of September 2019)

	3. Experience with high-performance computing and Linux environment is required
	4. Previous experience in molecular modelling (particularly ab initio simulations) is required
	5. Knowledge of computational and quantum chemistry is required
	6. Good writing and oral communication skills in English
Required documents:	1. CV and cover letter
We offer:	1. An opportunity to participate in a multidisciplinary project in one of the best scientific institutions in Poland
	2. Stimulating, young and friendly work environment
	3. Access to high-end computing equipment (CPU clusters)
Please submit the following documents to:	Please send your application to: trzask@cent.uw.edu.pl
Application deadline:	30.08.2019
FNP programme	

To allow us to process your data, please include the following statement in your application:

10. You have the right to lodge a complaint to the President of the Office for the Protection of Personal Data

11. Your application will be archived and stored for auditing purposes;

12. The name of the selected candidate/s will be made public on the CeNT UW website in accordance with the requirements of the funding agency.