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

JOB OFFER

Position in the project:	PhD Student
Laboratory:	Chemical and Biological Systems Simulation Lab
Scientific discipline:	chemistry
Keywords:	quantum chemistry, quantum embedding theories, molecular properties, heavy elements, relativistic effects, theoretical spectroscopy, non-covalent interactions
Job type (employment contract/stipend):	stipend
Part-time/full-time:	full-time
Number of job offers:	1
Remuneration/stipend amount/month:	5000 PLN gross gross
Position starts on:	01/04/2022 or soon after
Maximum period of contract/stipend agreement:	38 months, with the possibility of extension up to 45 months
Institution:	Centre of New Technologies, University of Warsaw
Project leader:	Małgorzata Olejniczak
Project title:	Embedding methods in quantum chemistry - pushing the boundaries of modeling molecular properties of complex systems with heavy elements.
Competition type:	SONATA BIS 10
Financing institution:	NCN
Project description:	The project involves interdisciplinary research on the boundary of computational quantum chemistry, applied mathematics, and data science, aimed at understanding of properties and behaviors of complex systems. The project aims to develop the methodology to calculate and analyze such systems, taking into account the presence of heavy elements and interactions with the environment. This methodology will be tested on a wide range of molecular complexes crucial for modern world applications (e.g.,

	environmental and pharmaceutical research).
Key responsibilities include:	Candidate will be involved in the following tasks: (i) quantum chemistry calculations of molecular properties in complex molecular systems with heavy elements exhibiting various types of intermolecular interactions and their analysis. These studies are aimed at assessing the quality of embedding methods for modeling molecular response properties arising from perturbations by mixed electric and magnetic fields. (ii) Participation in preparation of scientific publications. (iii) Active participation in group activities (seminars, tutorials).
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 Centre of Science for SONATA BIS-10 grant; Msc degree in chemistry or related discipline. The MSc degree should be obtained before the date of starting work in the project. - Confirmed status of a PhD student (on the date of starting work in the project at the latest). Other requirements: - basic knowledge of quantum chemistry - experience with quantum chemistry calculations is welcome, but not obligatory - ability to work in a group (possibility to work on-line), curiosity and motivation to learn, - willingness to work in interdisciplinary and international teams, - fluency in written and spoken english In practice: - we use quantum chemistry software – mainly DIRAC and ADF, - we do calculations on HPC clusters (Unix, Linux environments), - we write our own scripts and software (mostly in Python, Rust, Fortran), - we use Git, - we incorporate good practices in science (FAIR), good practices in creating and modifying software („extreme programming"),

	- we learn a lot from data scientists and software developer communities, - we use tools to make our work easier (to monitor tasks and projects (Notion), which also enables on-line work). The willingness to work in such environment is expected. Also, general interests in mathematics, data science and quantum chemistry, are very welcome.
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 employment in the project); 5. Signed information on the personal data processing, available from: https://cent.uw.edu.pl/en/wp-content/uploads/sites/5/2020/11/Information-clause_personal-data-processing.pdf
We offer:	- possibility to work in a newly established research group - possibility to work in international and interdisciplinary teams, - possibility to write an interdisciplinary PhD thesis in an actively developed research area, giving opportunities to work on theoretical (method development, software developments) and practical (computational modelling) research questions, - possibility to gain practical skills essential for future job market (data analysis, programming) - possibility to work on-line
Please submit the following documents to:	E-mail: malgorzata.olejniczak@cent.uw.edu.pl
Application deadline:	15/02/2022
Date of announcing the results:	15/03/2022
Method of notification about the results:	Email, website: https://cent.uw.edu.pl/en/career/