CeNT-27-2024

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 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:	Chemical sciences
Keywords:	Computation, biological assemblies, spectroscopies, drug delivery
Job type (employment contract/stipend):	stipend
Number of job offers:	2
Remuneration/stipend amount/month:	5000 PLN gross gross
Position starts on:	01/01/2025 or soon after
Maximum period of contract/stipend agreement:	36 months, with the possibility of extension up to 48 months
Institution:	Centre of New Technologies, University of Warsaw
Project leader:	Silvio Osella, PhD DSc
Project title:	Low-dimensional materials for solar fuels conversion and valorization (SOLAR2VAL)
Competition type:	NCN SONATA BIS 13
Financing institution:	NCN
Project description:	The goal of the project is to design stable and highly efficient hybrid nanomaterials for solar fuels generation, through an heterojunction structure in which absorption of light is followed by transfer of charges to the catalytic sites where the CO2RR and NRR take place to obtain ethanol, ethylene and ammonia as main products. The interface is based on low dimensional materials, focusing on 0D carbon dots, 2D layered materials and 2D catalysts such as 2D-MOFs and 2D-COFs. In this project we will use 1: multiscale computational methods to describe the chemical and physical properties of interfaces; 2: characterization of the charge transfer at the interfaces; 3: heterogeneous catalysis for CO2RR and NRR; 4:

	method development to compute the catalytic cycle in photo(electro)chemical environments. The computational part of the project will focus on 1. the rational design of low dimensional materials' building blocks by mean of ab initio computation to assess their opto-electronic properties. 2. Detailed study of the interfaces created by assembly different low dimensional materials, using a multiscale computational approach to fully assess the opto-electronic properties of the different interfaces in order to optimize charge or energy transfer processes. 3. In deep study of the heterogeneous catalytic cycle to obtain the desired products from CO2RR and NRR.
Key responsibilities include:	1. MD simulations of low dimensional materials' assembly. 2. Ab initio computation of absorption/emission properties of the constituents of the assembly. 3. QM/MM calculations and analysis of opto-electronic and transport properties. 4. Ab initio study on the heterogeneous catalytic cycle for the formation of solar fuels. 5. Analyses of the collected data. 6. Participation in preparation of scientific publications. 7. 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 NCN SONATA BIS 13.[1] We are looking for motivated people who have: - 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: - knowledge of quantum chemistry - experience with quantum chemistry calculations (ab initio and classical molecular dynamics simulations) - knowledge of simulation of low dimensional systems and experience with multiscale simulation approach (i.e. MD, CG, QM/MM, QM) is welcomed - 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

[1] Resolution of the NCN Council No. 50/2023 of 11 May 2023.

	In practice: - we use quantum chemistry software – mainly Gromacs, Gaussian and VASP - we do calculations on HPC clusters (Unix, Linux environments), - we write our own scripts and software (mostly in Python, bash, Fortran) for data analysis 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. At least two reference contacts (with phone numbers and emails) 6. Signed information on the processing of personal data
We offer:	- possibility to work in a newly established research group, -possibility to work in international and interdisciplinary teams, -stimulating and friendly work environment, attractive stipend, opportunity to work in an innovative international project, - possibility to gain practical skills essential for future job market, - possibility to work on-line
Please submit the following documents to:	E-mail: s.osella@cent.uw.edu.pl
Application deadline:	30/11/2024
Date of announcing the results:	15/12/2024
Method of notification about the results:	Email, CeNT UW website