

**CeNT-01-2025**

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

## JOB OFFER

Position in the project:	Student
Laboratory:	<i>Chemical and Biological Systems Simulation Laboratory</i>
Scientific discipline:	Chemical sciences
Keywords:	computation, charge and energy transfer, low dimensional materials, nano assembly, spectroscopy, heterogeneous catalysis
Job type (employment contract/stipend):	Stipend
Working time:	25-30 hours/week
Number of job offers:	1
Remuneration/stipend amount/month:	2000 PLN gross gross
Position starts on:	01.03.2025 or soon after
Maximum period of contract/stipend agreement:	24 months with the possibility of extension for a year
Institution:	Centre of New Technologies, University of Warsaw
Project leader:	Dr hab. Silvio Osella
Project title:	Low-dimensional materials for solar fuels conversion and valorization (SOLAR2VAL)
Competition type:	SONATA BIS 13
Financing institution:	NCN
Project description:	<p>The goal of the project is to design stable and highly efficient hybrid nanomaterials for solar fuels generation, through a heterojunction structure in which absorption of light is followed by transfer of charges to the catalytic sites where the CO<sub>2</sub>RR 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.</p> <p>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 CO<sub>2</sub>RR and NRR; 4: method development to compute the catalytic cycle in photo(electro)chemical environments.</p>



	<p>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 CO<sub>2</sub>RR and NRR.</p>
Key responsibilities include:	<ol style="list-style-type: none"><li>1. ab initio computation of absorption/emission properties of the light emitting molecules.</li><li>2. MD simulations of low dimensional materials' assembly.</li><li>3. Study of optical, electronic and transport properties from QM/MM calculations.</li></ol>
Profile of candidates/requirements:	<p>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 SONATA BIS 13 grant.</p> <p>Enrolled as a student of first cycle studies, second cycle studies or uniform Master's studies conducted in a higher education institution on the territory of Poland, in chemistry, physics or related discipline.</p> <p>Willing to spend 25-30 hours a week (flexible hours) to do interesting projects.</p> <p>With good oral/written communication skills in English.</p> <p>Although not required, any previous experience in molecular modelling would be welcome.</p>
Required documents:	<ol style="list-style-type: none"><li>1. Cover letter.</li><li>2. Current curriculum vitae.</li><li>3. Copy of document confirming the student status.</li><li>4. Signed information clause on the processing of personal data, available at: <a href="https://cent.uw.edu.pl/en/wp-content/uploads/sites/5/2020/11/Information-clause_personal-data-processing.pdf">https://cent.uw.edu.pl/en/wp-content/uploads/sites/5/2020/11/Information-clause_personal-data-processing.pdf</a></li></ol> <p>Before entering the competition, candidates are obliged to familiarise themselves with <a href="#">Internal Reporting Procedure</a>.</p>
We offer:	Stimulating and friendly work environment, attractive stipend, opportunity to work in an innovative international project.
Please submit the following documents to:	<a href="mailto:s.osella@cent.uw.edu.pl">s.osella@cent.uw.edu.pl</a>
Application deadline:	15.02.2025
Date of announcing the results:	25.02.2025
Method of notification about the results:	E-mail, CeNT website