## Ph.D. position within NCN SONATA BIS project

## Offer description

A 12-month PhD position starting on December 1, 2025, is available at the Institute of Physics, Nicolaus Copernicus University in Toruń, Poland, under the SONATA BIS Project No. 2021/42/E/ST4/00096 entitled *"Quantum Chemistry under Spatial Confinement"* (project leader: Dr. Szymon Śmiga).

Most of the research conducted within the project will focus on the efficient description of chemical and physical properties of many-electron systems under quantum confinement, in the context of both Wave Function Theory (WFT) and Density Functional Theory (DFT). Within the project, we will develop theoretical approaches and computational tools that enable the study of such systems. We will also concentrate on the development and validation of existing WFT and DFT methods. The PhD student will have the opportunity to carry out part of the project's tasks in collaboration with our international partner groups involved in the project.

## Benefits

We offer a monthly stipend of 4,500 PLN for a duration of 12 months. The successful candidate will join our highly experienced research team. Additional funds are available to support participation in 1–2 international conferences per year, as well as collaborative visits to our international partners in Italy and India.

## Eligibility criteria

***Offer Requirements***

REQUIRED EDUCATION LEVEL:

MSc in the field of physics, chemistry

REQUIRED LANGUAGES

ENGLISH: Excellent

## Skills/Qualifications

High motivation, excellent organization skills, openness to new knowledge and people, and acquisition of new skills. Good communication skills, including English proficiency. Good writing skills. Readiness to travel abroad.

## Specific Requirements

Training in the field of quantum mechanics and/or quantum chemistry
Knowledge about quantum chemical methods at the level of exchange and correlation effects
Knowledge about Density Functional Theory and Wave Function Theory methods

Very good programming skills (C++, Python will be more than welcome)
Experience with molecular quantum chemical codes (PSI4, PySCF will be more than welcome)

## Selection process

**Application documents:**

A complete application should include the following items: (in Polish or English)

1. A reference letter
2. Curriculum vitae (no more than two pages, A4 format) with a particular emphasis on academic achievements (scholarships, publications, patents, conference presentations, etc.)
3. Master thesis, or, if it is not completed or is not in English or Polish, the extended outline of the thesis.
4. Motivation letter explaining why the candidate is interested in the implementation of the project (the project abstract can be found in the attachments)

Please send your application documents directly to dr Szymon Śmiga **(szsmiga@umk.pl)**

**Application deadline 20.11.2025**

**Results: 26.11.2025**

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## Project description

The quantum confinement substantially alters the electronic structure of quantum systems (e.g. atom, molecules, and solids) as compared to their corresponding free state counterparts. This is exhibited in the changes in electronic energy levels, electronic shell filling, orbitals what, in consequence, affect their physical as well as chemical properties such as energetics, reactivity, response properties, etc. Therefore, the chemistry of confinement systems may drastically change. In recent years interest, both physicists and chemists in the study of the physical properties of confined quantum systems have increased with advances experimental techniques which allow to study e.g. atoms or molecules encapsulated in cages like fullerenes, nanotubes or zeolites, atoms, and molecules under pressure or quantum dots or simple molecules in quasi-2D or 2D regimes. The reduction of spatial dimensionality from three dimensions (3D) to 2D and 1D has been often used as an efficient strategy to promote the occurrence of new phenomena. Despite the large scientific effort on this topic, most of the studies and practically all applications have concerned confined extended systems, even if the practical realization of electronic confinement in chemical applications can also be achieved. The study of chemistry under electronic confinement is a challenging topic because the dimensional crossovers (from 3D to 2D and 1D) are one of the most difficult theoretical and computational problems.

One of the most crucial points when analyzing quantum confined systems is the choice of accurate model and quantum chemical method which allow to describe correctly the changes in the electronic wavefunction due to the effect of confinement. In recent years in most studies, the electronic wavefunction of the system subjected to confinement was span by a set of Gaussian-type orbitals

(GTO) belonging to the most widely utilized basis sets in the quantum chemical codes. This allows to study systems in soft confinement regimes by various wave function theory (WFT) and density functional theory (DFT) methods. The spatial electron confinement, in turn, is usually modeled by isotropic 3D, 2D, or 1D harmonic oscillator potential (with small oscillatory strength parameter ω) introduced to N-electron Hamiltonian. However, for larger values of confinement strength (strong quasi-1D/2D regime) or when harmonic potential becomes anisotropic, the common strategy is to supply standard GTOs with, specially designed anisotropic GTOs in order to guarantee that the wavefunction spans both Culombic and harmonic oscillator eigenstates. We note that these basis sets are not implemented in any of the popular codes, thus not allowing to routinely study of systems under various confinement with standard WFT and DFT methods. The first goal of the project is to implement the anisotropic GTOs in libint library what will allow their general utilization in novel quantum chemistry codes such as PSI4. Next, we will focus on the development and validation of existing WFT and DFT methods for the study of atoms, molecules, and molecular complexes subject to soft and strong spatial electronic confinement. Using accurate WFT methods (e.g. the coupled-cluster methods) we will create a database of confined chemical systems, which will be used to assess and improve the performance, and develop new, advanced DFT methods describing correctly the crossovers from 3D to 2D and 1D (second goal). We note, that most of the standard DFT methods fail badly in the description of dimensional crossovers mentioned before, thus not allow to model systems with strong quasi-2D or quasi-1D characteristics. The problem lays in the construction of the standard exchange-correlation energy functionals which cannot be used directly in low-dimensional regimes due to various limitations. Thus, the dimensional crossovers still remain one of the most difficult open problems in DFT.