Ph.D. position within NCN SONATA BIS project

Offer description

Four-year Ph.D. position starts **October 1, 2022**, available in the Institute of Physics Nicolaus Copernicus University in Toruń, Poland under SONATA BIS Project No. 2021/42/E/ST4/00096 entitled "***Quantum chemistry under spatial confinement***" (leader dr Szymon Śmiga).

Most of the research carried out within the project will focus on the efficient description of chemical and physical properties under quantum-confined in many-electron systems in the context of the Wave Function Theory (WFT) as well as on the Density Functional Theory (DFT). Within the project, we will develop the theory and tools allowing us to study such systems. We will also focus on the development and validation of existing WFT and DFT methods. The PhD student will have the opportunity to realize part of the project tasks in the groups of our international partners involved in the project.

Benefits

We offer 4500 PLN per month stipend for the whole duration of the PhD. The position is for 48 months. The successful candidate will be part of our highly experienced team. Additional funds are allocated to cover participation in international conferences (1-2 per year) and visits to international partners in Italy and India.

Eligibility criteria

Offer Requirements

REQUIRED EDUCATION LEVEL:

MSc in the field of physics, chemistry, computer science, astronomy

REQUIRED LANGUAGES

ENGLISH: Excellent

Skills/Qualifications

High motivation, excellent organization skills, openness to new knowledge, 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. Transcript of grades: diploma supplement, or the official transcript of grades, or, if they do not yet have these documents, grade book, or another document listing completed courses and grades. Information about the grading scale must be included;
4. Master thesis, or, if it is not completed or is not in English or Polish, the extended outline of the thesis.
5. 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 30.07.2022

Results: 10.08.2022

After the initial recruitment the applicant is required to submit their application to the online recruitment system of Exact Sciences and Life Sciences Doctoral School (AST NCU)

Work location:
1 position available at
Institute of Physics, Faculty of Physics,
Astronomy and Informatics,
Nicolaus Copernicus University,
Grudziądzka 5, 87-100 Torun, Poland

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.