Ph.D. position within NCN Preludium BIS-2 project

Offer description

Four-year Ph.D. position starts **October 1. 2021**, available in the Institute of Physics Nicolaus Copernicus University in Toruń, Poland under PRELUDIUM BIS-2 Project No. 2020/39/O/ST4/00005 entitled "***From Coupled Cluster theory to accurate semi-local Kohn-Sham correlation functional***" (leader prof. dr. hab. Ireneusz Grabowski).
Most of the research carried out as part of the project focus on the efficient description of the electron correlation effects in many-electron systems in the context of the Wave Function Theory (WFT) as well as on the Density Functional Theory (DFT) method in the Kohn-Sham (KS) implementation. The project aims to face the high numerical cost of *ab initio* type methods by developing new class density-dependent semi-local correlation functionals, compatible with orbital-dependent exchange-only OEPx/KLI/LHF functionals. This will allow applying a new class of methods to new, much broader problems in computational chemistry. All solutions will be implemented in state-of-the-art quantum chemical computational systems, e.g., ACESII and libxc library. Indeed, at the intermediate and final steps of this project, we will perform a detailed assessment of the newly developed methods by performing several tests for standard quantum chemistry benchmarks. The project will also allow for the search for new, more advanced methods describing correlation effects and the development of new functionals in both ab initio DFT and the standard KS-DFT. The Ph.D. student will have the opportunity to realize a part of the project tasks at the University of Nottingham, UK, during a planned foreign fellowship.

Benefits

We offer 5 000 PLN per month stipend to the month in which the mid-term evaluation of the doctoral student at the doctoral school is carried out, 6 000 PLN per month stipend after the month in which the mid-term evaluation of the doctoral student at the doctoral school is carried out. The position is for 48 months. The successful candidate will be part of our highly experienced team. Funds are allocated to cover participation in international conferences (1-2 per year) and for six months fellowship at the University of Nottingham, UK. The Ph.D. student is obliged to apply for funding for the fellowship at the University of Nottingham in the competition carried out by the Polish National Agency for Academic Exchange (NAWA) during his/her doctoral period at Doctoral school.

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 (the position requires a 6-month research stay in the UK)

Specific Requirements

Training in the field of quantum mechanics and/or quantum chemistry.
Basic knowledge about quantum chemical methods at the level of exchange and correlation effects
Basic knowledge about Density Functional Theory and Wave Function Theory methods
Basic knowledge about numerical methods. Basic knowledge of Linux, Python, C, Fortran 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 to Prof. Ireneusz Grabowski: **ig@fizyka.umk.pl**

Application deadline 30.07.2021

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 accurate description of the physical and chemical properties of ordinary matter (atoms, molecules, and solids) is a topic of extreme practical interest in a broad range of fields, including the development of smart materials, (molecular) electronics, biology, catalysis and many more. The accurate and efficient description of correlation effects in such systems is a long-lasting problem in the realm of quantum chemistry. Nowadays, there exist two main groups of quantum chemical computational methods, namely the wave function theory (WFT) and density functional theory (DFT) methods which trying to tackle this problem. Although the former approach is able to provide very accurate and reliable results their applicability for many large systems is still challenging due to very high computational cost. On the other hand, DFT methods, within the past few decades, have become a method of choice, especially due to its very attractive accuracy/computational cost ratio which allows applying it to many chemically and biologically important systems and solid state problems. The accuracy of DFT results is strictly related to the quality of so-called exchange-correlation (XC) density functional approximations (DFA) used in the DFT calculations. Currently, used ones benefit from the strong error cancellation effect between exchange and correlation parts of the functional. This, in general, leads to situations that we are getting the "right answers for the wrong reasons". There are many studies that report that both parts of standard density-dependent functionals do not describe correctly the effects assigned to their name e.g. the exchange functionals/potentials describes also the correlation effects etc. and vice versa. This is a quite big problem cause a number of physical and chemical quantities depend on the quality of XC potentials (related to XC functional through functional derivative) such as ionization potentials, electronic density and thus density-dependent quantities (e.g. dipole moments, etc.), excitation energies, etc. On the other hand, the utilization of the more accurate ab initio DFT approaches which in the physically correct manner describe both effects are still not often applicable in calculations due to large computational cost of correlation term. The naive combination of orbital dependent exact-exchange OEPx method with standard semi-local correlation leads to the worsening of the results. Thus, the main barrier to the widespread use of such methods is a lack of compatibility between these two types of functionals which is visible on the XC potential as well as density analysis.

The main aim of this project is to investigate the exact features of the correlation energy density CED and potentials from the CC method and to develop new, accurate semi-local correlation functional expression, compatible with OEPx method which will be able to provide the results beyond the current state-of-the-art. Thus, we will develop tools and methodologies aiming at increasing the accuracy of DFT method without increasing the computational cost. We note that the compatibility-based approach will be utilized for the first time in the context of functional development what gives this proposal definitely a pioneering nature. It is expected that this project will push the knowledge in the field beyond the actual limits enhancing significantly the applicative power of the DFT method, both in the chemistry and solid state physics. In fact, it is expected that the development of new accurate correlation functionals will allow within KS DFT to reach the accuracy of a CC method, at a much-reduced cost O(N^4) as compared to O(N^7). Thus, large systems for biology and nanoscience can be described with unprecedented accuracy. These achievements will have a relevant impact on the field of computational chemistry and physics.