Tytuł projektu

Ab initio DFT- praktyczne narzędzie dla chemii obliczeniowej

Project title

Ab initio DFT - practical tool for computational chemistry

Dyscyplina /Area of science

Nauki fizyczne

PROJECT DESCRIPTION

Research project objectives

The density functional theory (DFT) has become a method of choice in computational chemistry and in application to solid state physics, bio- and nanotechnology, as well as to atomic and molecular systems. This is due two reasons: I) very attractive accuracy/computational-cost ratio which allows applying DFT to very large molecular systems; ii) broad availability - implementations of such methods are already present in the vast majority of software packages for quantum-chemical calculations.

The DFT is an exact theory in principle, but in practice, the final quality of the results strongly depends on the approximations of the so-called exchange-correlation (XC) functional used in the Kohn-Sham DFT (KS-DFT) calculations. In general, the standard semi-local XC functionals give satisfactory results only in some areas of applications, and often the quality of the results obtained is not good enough and even unpredictable. Utilization of a more sophisticated, orbital-dependent functionals in the KS-DFT, constituting so-called *ab initio* DFT, lead to potentially an extremely powerful approach to electronic structure theory. Combining the efficiency of DFT with the accuracy and systematic improvement of wave function theory, it promises to bring computational chemistry to a new level, allowing the accurate description of the electronic properties. However, to date, this possibility is hindered by technical limitations that prevent the efficient and widespread use of *ab initio* DFT methods in computational chemistry applications. One of the main problems is related to the need to find a reliable and cheap basis set to expand the optimized effective potential (OEP), which is crucial for OEP method, another one is the effective implementation of the new OEP correlation functionals in KS-DFT methods.

In this project, which is directly connected to the phd student, we aim at facing these problems, in order to transform *ab initio* DFT into a really practical tool for computational chemistry. Thus, we will propose a solution to the long-standing problem of developing numerically stable OEP methods based on Gaussian basis sets. We will also implement a new version of the correlation functionals, which will allow applying *ab initio* DFT to new problems in computational chemistry.

Research methodology and preliminary plan

In order to transform *ab initio* DFT methods into a really practical tool (black box type) for computational chemistry we will develop different approaches to the basis set expansion of the OEP potential (necessary in solving integral OEP equations) using e.g. information from localized effective exchange-correlation methods, machine learning methodologies, regularization methods and also different approaches to the auxiliary and orbital Gaussian basis sets OEP implementation.

All solutions will be implemented in state of art quantum chemical computational systems e.g. ACES and/or PSI4. Next, they will be tested for systems for which accurate reference results are known. We will study the numerical stability of the methods, their basis set dependence, and implementation dependence. Additional research will also focus on the verification of the representation of the correlation effects by *ab initio* DFT and standard DFT correlation functionals, potentials, electron density and other properties like energy, IPs, reaction and atomization energies, enthalpies and more. In all above steps, phd student will be involved in conceptual work, running calculations and analyze of the results.

Expected impact of the research project on the development of science

The main practical purpose and anticipated effect of our research project are to **bring the DFT method to a new level of accuracy**. This would significantly increase the reliability of the results obtained in the framework of the DFT and the possibility of their application for the problems unattainable up to now to the standard DFT methods. Implementation of our new methods in computational packages will **allow transforming *ab initio* DFT methods into an efficient and powerful tool for computational chemistry available for the whole research community** especially computational chemists and physicists. The new methods will also allow for a better understanding of the description of correlation effects in the DFT approaches.

Required initial knowledge and skills of the PhD candidate

- Deep knowledge about quantum mechanics and quantum chemistry.
- Knowledge about quantum chemical methods at the level of exchange and correlation effects.
- Basic knowledge about Density Functional Theory and Wave Function Theory methods.
- Programming skills (FORTRAN, C, Python).
- Basis and/or advanced numerical methods knowledge.
- Using of artificial intelligence algorithms .
- Involvement in scientific work.

Zgłaszający projekt/ Author of the project

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Proponowani promotorzy i mentorzy/prospective supervisors

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