1. PHD PROJECT DESCRIPTION (4000 characters max., including the aims and work plan)

Project title: Effective construction of an accurate semi-local Kohn-Sham DFT correlation functional

1.1 Project goals

One of the biggest problems in Kohn-Sham (KS) density functional theory (DFT) is a lack of accurate semi-local exchange-correlation (XC) functionals that can be effectively used in KS calculations and in the same time provide reliable and accurate results. Currently used semi-local XC functionals benefits from the strong error cancellation effect between exchange and correlation parts of the KS functional. In general, this 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 numerous 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.
The main goal of the project is to derive the new, semi-local form of correlation functional which is compatible (no error cancellation effect) with the state-of-the-art exact exchange OEPx/KLI/LHF functionals and in the same time can provide the results which are comparable with *ab initio* wave function theory (WFT) approaches such as coupled-cluster (CC) method (i.e. CCSD(T)) at reduced computational scaling. To achieve this goal we will utilize two separate approaches:
• Up – down approach - starting from CC energy expression we will construct the correlation energy density (CED) from i.e. CCSD(T) method and develop new correlation functional using e.g. the Wigner-like CED expression
• Down – up approach – we will investigate the exact features of the correlation potential and develop new, and accurate semi-local potential and then (using linear path integral technique) construct the correlation functional

1.2 Outline

We will develop using a compatible-based approach the correlation functional/potential which is able to work together with the exact exchange OEPx method within KS framework. The construction will base on the analysis of the exact features of the CED and potentials obtained from the CCSD(T) method . Moreover, we will develop tools and methodologies aiming at increasing the accuracy of DFT method without increasing the computational cost.

1.3 Work plan

i. The WP1, that will run from the beginning to month 18th:
   - reconstruction of CED from CCSD(T) method for several atoms and molecules
   - construction of semi-local correlation functional mimicking the behavior of reference CC CED data
   - implementation in libxc and extensive testing

ii. The WP2, that will run from month 18th to month 36th:

- implementation of mRKS method and generation for several systems the real-space representation of the correlation potential
- mapping of reference correlation potentials onto a semi-local form
- reconstruction of correlation energy functionals from accurate model potentials by utilization of line integrals path technique
- implementation in libxc and extensive testing

iii. The WP3 (which will last from 30 month to the end of the project:
- application of the developed methods to some interesting problems in quantum chemistry and solid state physics e.g. calculation of ionization potentials, band-gaps and other solid state properties such as cohesive energy, bulk modulus, etc.

1.4 Literature

[1] R. J. Bartlett , I. Grabowski, S. Hirata, S. Ivanov, J. Chem. Phys. **122**, 034104, (2005)
[2] J. T. Margraf, et al. J. Chem. Phys. 150, 244116 (2019)
[3] S. Laricchia, et al. , J. Chem. Theory Comput. 2011, 7, 8, 2439-2451
[4] L. van Leeuwen et al. , Phys. Rev. A, 51 , 170, 1995

1.5 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.

1.6 Expected development of the PhD candidate's knowledge and skills

- Deep knowledge and understanding quantum-chemical methods ranging from *ab initio* (HF, CC, PT) up to DFT methods
- Acquiring extensive knowledge of description many-electron systems including electron correlation effects.
- Efficient programming at the advanced level, making parallel code, running quantum chemical calculations
- Ability to analyze the results and draw conclusions
- General knowledge about calculating different properties of many electron systems