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

Project title: Innovative methods for modeling electronic structures and properties of organic electronic molecules using electron pairs.

1.1. Project goals

Organic electronics is a promising technology for high-throughput manufacturing of eco-friendly, potentially low-cost, ultralightweight, flexible devices with various optoelectronic or electronic functionalities. The advancement of modern electronic devices can be accelerated by property optimization of its small building blocks, such as carbon-based molecules and polymer chains. We plan to use an unconventional electronic structure methods for efficient parametrization of the wave function to model large systems at low computational cost. An advantage over standard electronic structure methods is (a) the capability of reliable modeling long polymer chains often dominated by strong electron correlation effects and (b) the ability to compute orbital-based entanglement analysis (in terms of single orbital entropy and mutual information) to dissect orbital interactions and electron correlations in a given system.

1.2. Outline

In the proposed research project, we will further advance the pCCD group of methods to efficiently calculate charge transport properties in molecules important for organic electronics.
These include (a) the analysis of the locality of variationally optimized pCCD orbitals and (b) the design, implementation, and testing of pCCD-based models to calculate the charge transfer integrals efficiently.
All developments will be done in our locally developed PyBEST open-source software package [Comp. Phys. Comm. 264, 107933 (2021); Comp. Phys. Comm. 297, 109049 (2024)] and released to the public free of charge. The developed methodology will be used to model electronic structures and charge transfer properties of selected organic molecules essential for electronics.
These studies will be further augmented by entanglement analysis of orbital interactions to identify the conducting orbitals in the valence band. The project's outcome will allow us to reliably and efficiently model complex electronic structures and conducting properties of small building blocks and their aggregates beyond the limits of present-day quantum chemistry methods.
The developed quantum-chemical approaches will be directly applicable to other areas of chemistry, physics, and materials science, like the molecular design of semiconductors, organic light-emitting diodes, molecular wires, and organic batteries.

1.3. Work plan

- The design of new Python modules in the PyBEST software package
- Testing and implementation of charge-transfer models
- Quantum chemical calculations and results analysis
- The design of Graphical User Interface (GUI) using the Electron platform

1.4. Literature

- P. Tecmer, M. Gałyńska, L. Szczuczko, and K. Boguslawski, J. Phys. Chem. Lett., 14, 9909-9917 (2023)
- K. Boguslawski, A. Leszczyk, A. Nowak, F. Brzęk, P. Sz. Żuchowski, D. Kędziera, and P. Tecmer Pythonic Black-box Electronic Structure Tool (PyBEST). An open-source Python platform for electronic structure calculations at the interface between chemistry and physics, Comp. Phys. Comm., 264, 107933 (2021)

1.5. Required initial knowledge and skills of the Ph.D. candidate:

-basic knowledge of Python, git, GitLab, and Latex
-basic knowledge of organic chemistry

-good knowledge of quantum physics/chemistry
-good knowledge of English
-experience with Linux/Unix and computer clusters

1.6. Expected development of the Ph.D. candidate's knowledge and skill

-high-quality programming skills and a co-authorship of the PyBEST software package
-version control (git) and continuous integration (GitLab)
-expert knowledge of the electronic structure methods
-state-of-the-art computational modeling of electronic structures of organic photovoltaic materials and their properties
-improved soft and hard skills (presentations, reports, communications, working in the team)