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

Project title: Modelling electronic structures and charge transfer properties of small building block of organic electronic materials

1.1. Project goals

The efficient operation of organic electronic devices requires organic semiconductors with high charge mobility. Hence, searching for high-mobility organic semiconductors is important for new organic solar sales (OSC) and light-emitting diodes (OLEDs). Currently, the research for optimal organic building blocks relies on a trial-and-error approach, which is expensive and time-consuming. A reliable quantum chemistry-assisted screening of small building blocks of organic semiconductors can unveil the relationship between chemical structure and charge mobility and speed up technological advancement. The proposed Ph.D. research project aims at developing efficient and reliable computational protocols for quantum chemical modeling of charge transport properties in organic molecules. Specifically, standard electronic structure methods and unconventional approaches based on geminal theories are going to be investigated. The latter will be augmented with the quantum information analysis of orbital interactions and electron correlation patterns.

1.2. Outline

- Assess the performance of various charge transfer models (e.g., based on Markus and Landau-Zener theories)
- Quantum entanglement analysis of small and medium-sized building blocks of organic solar cells
- Prediction of charge transfer properties, guide for experimental manipulations

1.3. Work plan

- Mathematical analysis of charge-transfer models
- generation of reference data
- implementation of charge-transfer models in PyBEST
- large-scale modeling with PyBEST

1.4. Literature

- Newton, M. D. Chem. Rev. 1991, 91, 767–792.
- P. Tecmer, M Gałyńska and K. Boguslawski, J. Phys. Chem. Lett., 14, 9909-9917 (2023))
- P. Tecmer, K. Boguslawski “Geminal-based electronic structure methods in quantum chemistry. Toward a geminal model chemistry.”, Phys. Chem. Chem. Phys. 24, 23026-23048 (2022)
- K. Boguslawski, A. Leszczyk, A. Nowak, F. Brzęk, P. Sz. Żuchowski, D. Kędziera, and P. Tecmer, Comp. Phys. Comm., 264, 107933 (2021)

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

- analytical thinking
- good knowledge of English-good knowledge of English
- Python
- PyBEST software package
- Physical and organic chemistry

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

- high-quality scientific papers where the Ph.D. student is the first/leading author
- co-authorship in the PyBEST software package
- proficiency in Latex, git, GitLab, ruff, GitLab CI
- understanding of electronic structure and properties of large organic molecules
- large-scale modeling of organic electronics with modern quantum chemistry software packages
- high-performance computing skills, including GPU cards