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

Project title: Novel quantum chemistry approaches for modeling charge transfer properties in organic electronics.

1.1. Project goals

Organic electronics represent an eco-friendly, flexible, and potentially low-cost alternative to traditional electronics. The efficient operation of organic electronic devices requires organic semiconductors with high charge mobility. Hence, the search for high-mobility organic semiconductors is of predominant importance. Up to date, this search heavily relies on a trial-and-error approach, which is expensive and time-consuming. A reliable quantum chemistry-aided screening of the plethora of organic semiconductors can make their optimization process more efficient and unravel precious information about the relationship between chemical structure and charge mobility. Unfortunately, the size of the organic molecules and materials in question prohibits the use of wave-function-theory (WFT)-based methods. To that end, the quantum chemical modeling of electronic structures and properties of organic semiconductors and devices commonly relies on density functional approximations (DFAs) and semi-empirical approaches. These are cost-effective methods but do not always provide physically reliable results as many of the long polymer chains, common building blocks of organic electronic devices, exhibit quasi-degeneracies and feature electronic structures of multi-reference nature. The proposed research project will change the present computation paradigm by developing efficient and reliable models for predicting charge transport properties in organic molecules. Our goal will be achieved with unconventional electronic structure methods that use a compact parametrization scheme of the electronic wave function, namely pair-coupled cluster doubles (pCCD)-based approaches.

1.2. Outline

The developed charge transfer models will be implemented in our open-source quantum chemistry software package PyBEST. Specifically, these include:

- The design, implementation, and testing of charge transfer models.
- The design and implementation of a graphical user interface in the cross-platform Electron framework.
- Large-scale quantum chemical modeling of polyaniline and its derivatives combined with a quantum entanglement and correlation analysis of their electronic structures.

1.3. Work plan

- literature study of modern charge-transfer models
- quantum chemical modeling of electronic structures and properties of small components of OPV materials
- generation of reference data for charge-transport models
- implementation of charge-transfer models in PyBEST
- large-scale modeling of charge-transport properties of model organic electronic materials using PyBEST

1.4. Literature

- Newton, M. D. Chem. Rev. 1991, 91, 767–792.
- Risko, C, McGehee, M. D., Brédas, J.-L. Chem. Sci., 2, 1200–1218 (2011)
- 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)
- Boguslawski K., Tecmer P., Ayers P.W., Bultinck P., De Baerdemacker S., Van Neck D. Phys. Rev. B 2014, 89, 201106(R)

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

-enthusiasm for science and commitment to hard work
-analytical thinking
-good knowledge of English
-basic knowledge of quantum physics and/or chemistry
-basic knowledge of Linux/Unix, computer clusters, and modern programming languages (such as Python and C++)

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

-scientific independence
-high-quality programming skills
-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
-co-authorship in the PyBEST software package
-improved soft and hard skills (presentations, reports, communications, working in the group)
-experience in writing grant applications
-good quality scientific papers, where the Ph.D. student is the first/leading author