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

Project title: Advancement of pCCD-based methods to modeling electronic structures and properties of organic solar cells

1.1. Project goals

The ultimate goal of the proposed research project is the large-scale modeling of electronic structures and properties of small building blocks of organic photovoltaic materials using unconventional electronic structure methods and model Hamiltonians. This goal will be achieved by employing the Antisymmetric Product of 1-reference orbital Geminal (AP1roG), also known as the pair Coupled-Cluster Doubles (pCCD), and its extensions. The advantage of these approaches over the standard quantum chemistry methods is their ability to reliably account for strong electron correlation effects even in large molecular systems. That is particularly beneficial for describing electronic structures of many OPVs building blocks, where the multi-reference or biradial nature limits the applicability of standard electronic structure methods such as Density Functional Theory.

1.2. Outline

The efficiency of OPVs, typically composed of conjugated polymers as donors and fullerene derivatives as acceptors, is strongly related to the offset between the donor's highest occupied molecular orbital (HOMO) and the acceptor's lowest unoccupied molecular orbital (LUMO) as well as the characteristic features of low-lying electronic transitions. While it is highly desirable to tune such properties theoretically at the quantum level, the molecular size of OSCs prohibits the use of the most reliable and commonly available methods. To remedy this problem, we will use and further advance some of the most promising unconventional quantum chemistry methods, which feature more favorable computational scaling, and thus are capable of modeling large molecules. The acquainted knowledge about the electronic structures and properties of selected organic compounds will then be used to parameterize model Hamiltonians to extend the applicability of the theoretical model to even larger systems. Such an original approach will be developed in our locally developed, open-source PyBEST software package, opening the way for a reliable quantum chemical description of OPVs for the first time.

1.3. Work plan

-literature study of modern OPV structures and properties and data collection
-choice of optimal orbitals for pCCD
-dispersion correction models on top of pCCD
-quantum chemical modeling of electronic structures and properties of small components of OPV materials
-generation of reference data for small building blocks of OPVs
-the creation of a unique data set of electronic structures and properties of OPV components
-parametrization and testing of model Hamiltonians in PyBEST s
-large-scale modeling of OPVs electronic structures and properties with model Hamiltonians.

1.4. Literature

-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