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

Project title: Eclectic theoretical design of novel light-harvesting materials

1.1. Project goals

- benchmark studies to assess the accuracy of pCCD-based methods in describing and predicting molecular properties of small OSC model systems
- accurate and efficient prediction of the properties of OSCs of various sizes, ranging from small building blocks to large π-extended systems

1.2. Outline

The advancement of light-harvesting materials and highly-efficient electroluminescent devices is of growing importance in both academia and industry. However, in order to compete with other (photovoltaic) technologies, further improvements are still desirable. This can be achieved by means of more reliable quantum chemical predictions of electronic structures and properties of modern materials. Yet, the size of common OSC components prohibits the use of standard wave-function methods, whereas DFT might fail due to their MR nature. Because of their efficiency and good performance, pCCD-based methods can be employed to, for instance, effectively screen and group various OSC motifs, providing a one-of-a-kind data set library for the future development of electronic devices, and predict (not simply reproduce) experimental data that can be exploited in molecular design. Thus, this project may shift the current paradigm in computational chemistry, large-scale modeling, and theoretical materials design towards novel and systematically improvable approaches (beyond DFT) implemented in modern quantum chemistry codes that use progressive programming models. Furthermore, the outcome of the project can provide a reliable database of OSCs for machine learning.

1.3. Work plan

The proposed PhD project includes the following work tasks:

- Benchmark study of OSCs using pCCD-based methods (ground and excited state electronic structures as well as their properties, like dipole moments)
- Reference calculations using highly-accurate wave-function based methods, like DMRG, DMRG-tailored CC, and EOM-CC.
- Molecular Engineering of modern organic solar cells
- Large-scale modeling of building blocks of organic electronic devices (donor and acceptor molecules from the HOPV15 dataset as well as novel fulvene-derivatized fullerenes)
- Modeling the HOMO-LUMO using the extended Koopman's theorem

1.4. Literature

- Molecular Electronic-Structure Theory, T. Helgaker, P. Jørgensen, and J. Olsen, John Wiley & Sons, New York, 2000.
- Many-Body Methods in Chemistry and Physics, MBPT and Coupled-Cluster Theory, I. Shavitt and R. J. Bartlett, Cambridge University Press, Cambridge, 2009.

- A. Leszczyk, P. Tecmer, and K. Boguslawski (2019) New Strategies in Modeling Electronic Structures and Properties with Applications to Actinides. In: Broclawik E., Borowski T., Radoń M. (eds) Transition Metals in Coordination Environments, vol 29. Springer, Cham.

1.5. Required initial knowledge and skills of the PhD candidate

- Basic knowledge of molecular electronic structure theory like Hartree-Fock theory, multiconfigurational self-consistent field theory, coupled cluster theory, etc.
- The candidate should be familiar with Linux, bash, and basic terminal commands
- The candidate should be fluent in spoken and written English (the project language will be English)

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

- The candidate will gain expertise in unconventional electronic structure methods, like the density matrix renormalization group algorithm, geminal-based wave function ansätze, and various coupled cluster flavors
- The candidate will gain fundamental knowledge in state-of-the-art many-body-theory for ground and excited states for both closed- and open-shell systems
- The candidate will be actively involved in software development of our own open-source software package written in Python and C++ (using the version-control system git and GitLab).
- The candidate will be well trained in electronic structure calculations (using wave function based methods) at various scales