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

Project title: Devising Reliable Electronic Structure Schemes through Eclectic Design to Model Light-Harvesting Materials

1.1. Project goals

- Improving ground and excited state pCCD through eclectic design to be applicable to model light-harvesting materials
- Improving ground and excited state post-pCCD methods through eclectic design to be applicable to model light-harvesting materials
- Extending the derived models to open-shell electronic structures

1.2. Outline

Experimental studies on the advancement of photovoltaic materials heavily rely on a trial-and-error approach. This disadvantage entails large workloads and depletes a lot of time and consumables. A more efficient approach is to exploit quantum chemistry to guide the synthesis of new materials and accelerate the development of novel compounds. The computational models, however, are difficult primarily because conventional highly-accurate approaches are technically limited to small model compounds and demand user control on an expert level. In large-scale modeling of new materials, DFT is hence considered as the method of choice. Yet, DFT may predict unreliable electronic structures and molecular properties as heavy-element containing organic electronics may feature a substantial amount of strong correlation. In this project, we will develop innovative hybrid wave-function-based approaches that are designed to be computationally inexpensive, robust, and black-box-like, requiring minimal user–software interplay. The proposed models will be implemented in PyBEST and will (i) enhance our fundamental understanding of molecules and their properties, (ii) aid the development of black-box quantum chemistry calculations, and (iii) accelerate the discovery of new materials. Thus, this project will shift the current paradigm in computational chemistry, large-scale modeling, and theoretical materials design of organic electronics towards novel and systematically improvable approaches (beyond DFT).

1.3. Work plan

The proposed PhD project includes the following work tasks:

- Tuning of ground-state pCCD (with and without orbital optimisation)
- Tuning of ground-state post-pCCD models
- Extending the open-shell extension for the improved pCCD-based methods
- Extending the electronically excited state models for the improved pCCD-based methods

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