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

Project title: Eclectic design of quantum many-body theory

1.1. Project goals

- Design of novel, hybrid electronic structure methods that are applicable across the periodic table for both ground and excited states
- Extension of the new methods to open-shell compounds
- Application of the proposed quantum mechanical models to i) small model systems used for benchmark calculations and ii) production runs for molecular properties of organic light emitting diodes (OLEDS)

1.2. Outline

Modern quantum-many-body theory has reached a remarkable level of description of atoms and molecules and their interactions. Unfortunately, conventional state-of-the-art theoretical models are difficult primarily because the computational resources required grow exponentially with the size of the system. To break the exponential-scaling wall of present-day methods, novel and neat approximations are desirable. One such innovative approach models many-electron systems as collections of non-interacting electron pairs, so-called geminals. In this project, we aim at improving current geminal-based models by dressing electron-pair states with information extracted from multi-reference wave functions. The proposed models will thus combine the strengths of different conventional and unconventional electronic structure methods in a synergistic manner resulting in reliable, inexpensive, and black-box-like approaches.

1.3. Work plan

The proposed PhD project includes the following work tasks:

- Derivation of the working equations of dressed geminal-based models
- Implementation, testing and debugging, code optimization and parallelization
- Benchmark calculations for well-known strongly-correlated systems
- Derivation of N-particle RDM from the dressed geminal models
- Analysis of the dressed geminal models using concepts of quantum information theory, like the single-orbital entropy and the mutual information
- Production runs to investigate molecular properties of OLEDS
- Performing reference calculations using state-of-the-art methods, including literature searches for reference data

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

- Basic programming skills in modern languages are mandatory (like Python and/or C++)
- 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 flavours
- 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 enhance his/her mathematical skills as all working equations for the above mentioned theoretical models have to be derived
- The candidate will be actively involved in software development of our own open-source software package written in Python, C++, and Fortran (using the version-control system git and GitLab). This includes implementation, testing, debugging, optimization, parallelization, benchmarking, and maintenance.
- The candidate will be well trained in electronic structure calculations (using wave function based methods) at various scales