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

Project title: Towards a reliable and efficient description of electron correlation effects in large molecules: embedding pCCD-type methods

1.1. Project goals

-development of one-of-a-kind WFT-in-DFT models based on pCCD-type wavefunctions
-code optimization and GPU support in the PyBEST software package
-the ultimate goal of the proposed research project is the-reliable modeling of large molecular systems based on these unique WFT-in-DFT models using supercomputers

1.2. Outline

The Ph.D. project focuses on embedding pCCD-type wavefunctions in Density Functional Theory (DFT). In this way, the efficiency of DFT is combined with the reliability of pCCD-based methods in modeling the electronic structures of large molecules. The Ph.D. candidate will have the opportunity to implement several variants of embedding methods in our local software package PyBEST, test their performance and reliability. The newly developed models will be applied to challenging problems in quantum chemistry, ranging from some model systems to actinide species. Examples are large assemblies of early actinide oxides forming the so-called cation-cation interaction complexes.

1.3. Work plan

-literature studies and data collection
-design and implementation of the static and exact embedding models in the PyBEST software package
-testing, benchmarking, code optimization and reprogramming bottle-neck operations on GPUs in the PyBEST software package
-application of above-mentioned models to challenging problems in quantum chemistry
-code release

1.4. Literature

-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)
-Q. Sun and G. K.-L. Chan, Quantum Embedding Theories, Acc. Chem. Res. 49, 2705-2712 (2016)
-P. Tecmer et al. Assessing the Accuracy of New Geminal-Based Approaches, J. Phys. Chem. A , 118, 9058-9068 (2014)

1.5. Required initial knowledge and skills of the PhD 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, modern programming languages (such as Python and C++)

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

-scientific independence
-high-quality programming skills (Python, C++, and CUDA)
-version control (git) and continuous integration (gitlab)
-expert knowledge on the electronic structure methods
-state-of-the-art computational modeling of electronic structures of large quantum systems
-advanced usage of computer clusters and software maintenance
-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 (or leading) author