Tytuł projektu
Nowoczesne metody zagłębiania kwantowego służące do modelowania wydajnych organicznych ogniw fotowoltaicznych
Project title
Modern quantum embedding approaches for the design of efficient organic photovoltaic materials
Dyscyplina /Area of science
Nauki fizyczne
PROJECT DESCRIPTION

The proposed research project aims at developing new, robust, computationally inexpensive, and reliable quantum chemical models to aid the design of new efficient organic photovoltaic compounds. Organic photovoltaic materials represent a cheaper alternative to currently used inorganic solar cells, but have lower quantum efficiency and often undergo uncontrolled oxidation and reduction resulting in fast degradation and decrease of performance over time. To that end, their intrinsic electronic structure properties need to be further modified. Since experimental manipulations with possibly large amount of organic compounds is very time consuming, optimization of the new and promising organic photovoltaic compounds can be more efficiently done with computer simulations at the quantum level. Unfortunately, the size of many new candidates and encouraging compounds for organic photovoltaics prohibits the use of reliable, but expensive quantum chemistry methods. Thus, new hybrid quantum chemistry approaches are needed. This will be achieved by coupling efficient and reliable geminal-based methods with Density Functional Theory (DFT) using Wave Function Theory (WFT)-in-DFT embedding techniques. To accomplish this task, additional features must be incorporated into the quantum mechanical model. These include systematically improvable WFT-in-DFT embedding techniques such as (i) a static embedding potential, (ii) embedding with an imposed (approximate) orthogonality condition for the subsystems, and (iii) the so-called exact embedding potential. All proposed WFT-in-DFT models will be implemented in our locally developed open-source quantum chemical software package PIERNIK (Python-based). To accelerate code performance, the most expensive numerical operations, will be either rewritten in C++ exploiting conventional math libraries, or adopted to the modern GPU (Graphics Processing Unit) architecture. To enhance WFT-in-DFT convergence, the separation between the system (the part described by WFT) and the environment (the part mimicked by DFT) will by guided using concepts of quantum information theory.

Reliable quantum chemical modeling of electronic structures can be particularly instructive for describing molecules and materials that are difficult to manipulate experimentally because they are unstable or toxic. Conventional electronic structure methods, however, are also difficult, primarily because they are technically limited to small model compounds and typically demand user control on an expert level. The proposed theoretical embedding models are designed to be computationally inexpensive, robust, and black-box-like, lowering the user-software interplay as much as possible. Moreover, the proposed innovative entropy-based partitioning scheme will pave the way to a black-box-like partitioning protocol, one of the main concerns of embedding theories. Specifically, the developed novel partitioning approach combined with inexpensive, new WFT-in-DFT flavors will be essential to accurately tune the separation between the Highest Occupied Molecule Orbital (HOMO) and the Lowest Unoccupied Molecular Orbitals (LUMO) and related properties of new organic materials. Finally, the proposed embedding methods will be directly applicable to other challenging areas of physics, chemistry, and materials science.

Required initial knowledge and skills of the PhD candidate

- ➔ Analytical thinking
- ➔ High motivation for work and scientific development
- ➔ Understanding of basic physics, chemistry, and quantum mechanics
- ➔ Basic knowledge of linux operating system, Latex, and modern programming languages (e.g., python and C++)

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