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Title: **Novel hybrid computational chemistry methods for the design of efficient organic photovoltaic materials**

The proposed research project aims at the development and application of new, robust, computationally inexpensive, and reliable quantum chemical models to aid the design of new efficient organic photovoltaic compounds. Modern Organic PhotoVoltaic (OPV) materials represent cheaper and more environmental friendly alternatives to the commonly used inorganic solar cells. The lower Power Conversion Efficiency (PCE) in OPVs is overcompensated by their flexibility, simple assembly technology, and their light-weight allowing us to build effectively large-scale light-harvesting devices even on difficult surfaces. The OPV deficiencies, such as the lower PCE as well as uncontrolled oxidation and reduction processes that cause a fast degradation and decrease of the performance over time, are currently active fields of research. Both theoretical and experimental studies are the source of new OPV materials with more and more efficient PCE parameters and higher resistance to degradation. One way to advance the design and developments of new OPV materials and device architectures is to better understand the physical and chemical processes behind the generation of the photo-current. Since experimental manipulations with possibly large amount of organic compounds are very time consuming, the optimization of new and promising organic photovoltaic compounds can be more efficiently done with computer simulations at the quantum level. The effective synergy between theoreticians, who indicate molecular candidates for synthesis and further experimental investigations, combined with a reliable description of their electronic structures will shed a new light on the field of novel OPV materials.

Unfortunately, most of the new promising candidates for OPV compounds are too large to be modeled with reliable wave function theory (WFT) quantum chemical methods. The solution to this problem comes with hybrid approaches, where Density Functional Theory (DFT) is combined with the WFT part via so-called embedding techniques. In this approach, the active side of the molecules is represented by reliable, but time consuming WFT methods, while the remaining part, often called the environment, is represented by the less accurate, albeit much cheaper DFT method. In the proposed research project, the aim will be set on developing efficient and reliable approaches to model electronic ground and excited state properties and their application to both already existing and hypothetical OPV materials and their small building blocks. Specifically, we will focus on polymers with low-optical gaps.