The decarbonization of the energy sector is one of the major challenges in the XXI century in the context of limiting climate change while rapidly developing the global economy and increasing world population. Renewable energy sources will play a key role in the transformation of the energy sector and will cover 86% of global energy consumption by 2050. Sunlight has by far the highest theoretical potential of all known earth's renewable energy sources. There is more solar energy striking the earth's surface in one and a half hours than global energy consumption in 2001 from all sources combined. Such tremendous potential of solar energy provided a great driving force for the research in photovoltaics in the last 50 years, which resulted in the development of new technologies and significant improvements in solar cell efficiencies.

Despite the considerable development, all standard single-junction solar cells share the same fundamental loss mechanisms that limit their theoretical efficiency to 33%, the Shockley-Queisser limit. The major loss of approx. 30% can be attributed to thermalization, which is the loss of excess energy above the bandgap of the solar cell after the absorption of a high-energy photon. Theoretical studies predict that utilizing singlet fission in solar cells can increase their theoretical maximum efficiency up to 45%. Singlet fission is a photophysical process where molecules excited upon absorption of one high-energy photon evolve into two triplet excited states, which can be extracted as two electrons. Large-scale application of singlet fission in photovoltaics requires a good understanding of this process, which was the driving force for a number of mechanistic investigations in the past decade. Despite that, there are still important questions to be answered, such as what is the impact of intermolecular arrangement in three-dimensions; how to efficiently harvest triplets generated in singlet fission; what is the role of conformations and vibrations; or how entropy activates the formation of high-energy triplets.

Answering urging questions regarding singlet fission requires new molecular architectures. In this project, we propose three molecular strategies specially designed to answer some of the remaining questions essential to fully establish the structure-property relationships. The answers are important for the design of ideal singlet fission materials. The first two strategies will focus on systematic studies on intermolecular distance relationship with singlet fission efficiency. This is crucial because it will help to precisely design the bulk material properties. The third research avenue will concentrate on the delocalization of excited states formed upon singlet fission, hence, on entropic contribution to the activation of endothermal singlet fission. This is an extremely important issue because entropic activation might enable harvesting high-energy triplets, which will make singlet fission compatible with widely used silicon solar cells.

The proposed structures will be synthesized and initially characterized by the project group members at the Institute of Organic Chemistry of the Polish Academy of Sciences in Warsaw. Detailed photophysical studies will be done in collaboration with expert spectroscopy groups of Prof. Jacek Waluk from the Institute of Physical Chemistry of the Polish Academy of Sciences and Prof. Dirk Guldi from Friedrich Alexander University Erlangen-Nurnberg in Germany.