"Hybrid Materials for Efficient Energy Generation and Information Technologies"

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Title: Exciton Diffusion in Hybrid Solar Cells – *A Theoretical Challenge*

Hybrid solar cells combine inorganic and organic semiconductors with tailored properties. Organic semiconductors have very high absorption coefficients, which makes some particular suited as the main light-absorption species in these hybrid devices. Therefore, knowledge about the fate of excitons generated on the organic component is of crucial importance for the understanding and further optimization the device structure and composition. But while charge transport in organic semiconductors has been widely studied, exciton diffusion is only poorly understood. This is particularly true for conjugated polymers, where exciton diffusion is typically limited to a 5-15 nm length scale.

The aim of the project is to perform in-depth theoretical investigations (PhD-2) of exciton diffusion from a theoretical perspective on the electronic scale. This is a challenging but very rewarding task requiring an enthusiastic PhD candidate. Based on (time-dependent) density-functional theory and many-body perturbation theory, a method shall be developed to study propagation and de-excitation of an optically excited system thereby also accounting for structural relaxation. The outcome of this theoretical work will be related to the results of extensive experimental studies on structurally well-defined hybrid layer systems.

With this combined theoretical-experimental knowledge, we hope to get a comprehensive understanding of the processes which determine the exciton diffusion length in conjugated materials as part of a hybrid solar cell device. The outcome of these studies will not only lead to a better understanding of the function of hybrid solar cells, but allow more general conclusions regarding then migration of energy in conjugated organic materials