PhD Project description, M.Sc. Michael Adams

Ultrafast time-resolved spectroscopy

The design of specific, desired energy transport characteristics into advanced synthetic materials is still in its infancy. Organic semiconductors, surface anchored metal organic frameworks (SURMOFs), and lead halide perovskites are of broad interest in a wide variety of applications across the fields of nanotechnology, photonics, microelectronics, and optoelectronics. In these applications, both established and emerging, incomplete control of energy flow on the nanoscopic level limits macroscopic device performance. Ultrafast time-resolved spectroscopy has played a key role in reaching the current understanding of the fundamental physics underpinning the device-relevant characteristics of these materials. However, significant gaps in the understanding remain. This project will close these gaps, studying the photophysical loss mechanisms that environmental degradation causes in organic solar cells and developing pump-probe spectroscopic methods that allow transient electric fields to be observed in perovskite and SURMOF solar cells (in the 50 fs to 4 ns ultrafast time window). This will significantly aid the further development and design of organic semiconductors, metal-organic-frameworks, and perovskites for solar cell applications. Three main research questions can be formulated:

I. What are the photophysical effects that lead to decreased solar cell performance caused by aging of organic solar cells?

- Many factors have been reported to affect the stability of OPVs. These include exposure to light, temperature and environmental factors such as oxygen and humidity. To understand how to circumvent the effects of these degradation causes, it is important to elucidate the mechanisms by which they affect the fundamental photophysical processes in the device active layer and thus, the device performance.
- In a Heika funded project, Prof. Vaynzov at the University of Heidelberg will prepare and encapsulate organic solar cells that have been aged under controlled conditions. We will then perform transient absorption and Streak camera measurements on these devices to ascertain the effect of specific degradation mechanisms on the photophysical processes occurring in the device.

II. Can we understand charge separation in surface anchored metal organic framework (SURMOF) and lead halide perovskite solar cells by time-resolved observation of the photoinduced Stark effect?

- Recently, novel SURMOFs have been developed that operate as the active layer of a solar cell. It is unclear how charge separation proceeds following photon absorption in these exciting new materials. These materials and devices will be made in collaboration with the Institut für Funktionelle Grenzflächen (IFG). Currently the first generation of materials can only convert blue light into electricity. Extending the ability of these devices to harvest more of the solar spectrum will be a goal of this project.
- Lead halide perovskite solar cells have revolutionized the solution-processable thin-film photovoltaic research community over the last 2 years, with power conversion efficiencies of 20% almost doubling that of their competitors. We will receive perovskite solar cells through the PERSOL BMBF project through collaborators in Darmstadt (Prof. Jägermann) and at LTI (Prof. Lemmer). These will have controlled crystal grain sizes, ranging from millimeter scale single crystals to polycrystalline films with nanometer sized grains. Studying these will reveal the roles of bulk and grain boundaries in the solar cell performance.
- The separating charges induce a change in absorption in the material in their local environment. We will develop the capability to measure this effect with transient pump-probe spectroscopy. This will allow us to understand the initial charge separation event happening on the sub-nanosecond timescale, which is highly relevant information for the design of next generation materials.

III. Can similarly efficient charge generation (as in II) be achieved in lead-free perovskite materials and in SURMOFs that absorb more of the solar spectrum?

- As the PERSOL project progresses, the shift will be to develop lead-free materials to replace the lead halide perovskite in the solar cell. We will apply our techniques and knowledge of the lead halide system to determine whether these materials satisfy the fundamental requirements to perform in the solar cell, and if not, what needs to be improved.
- Similarly, as we aid in the development of redder absorbing dyes for the photovoltaic SURMOFS, we will continue to investigate how quantum efficiencies can be kept high, and how the materials can be made to function by monitoring the fundamental photophysical processes.