Molecular Dynamics in Organic Solar Cells

Besides the development of new organic solar cells with the goal of improving their performance as photovoltaic devices, environmental stability and ecological compatibility, our group is particularly dedicated to various experimental methods, especially scattering techniques, in order to understand the basic properties of the applied materials and built devices. A key tool for the investigation of dynamics on a molecular level in polymers and polymer blends/solutions is quasielastic neutron scattering (QENS). Our group is involved in the cold neutron time-of-flight spectrometer TOFTOF (FRM II, Garching),[1] which offers broad possibilities for QENS measurements. A schematic picture of the instrument, which sows the chopper system (c) as well as the neutron beam (a) and the detector array (f) around the sample position (d), is shown in *Figure 1*.

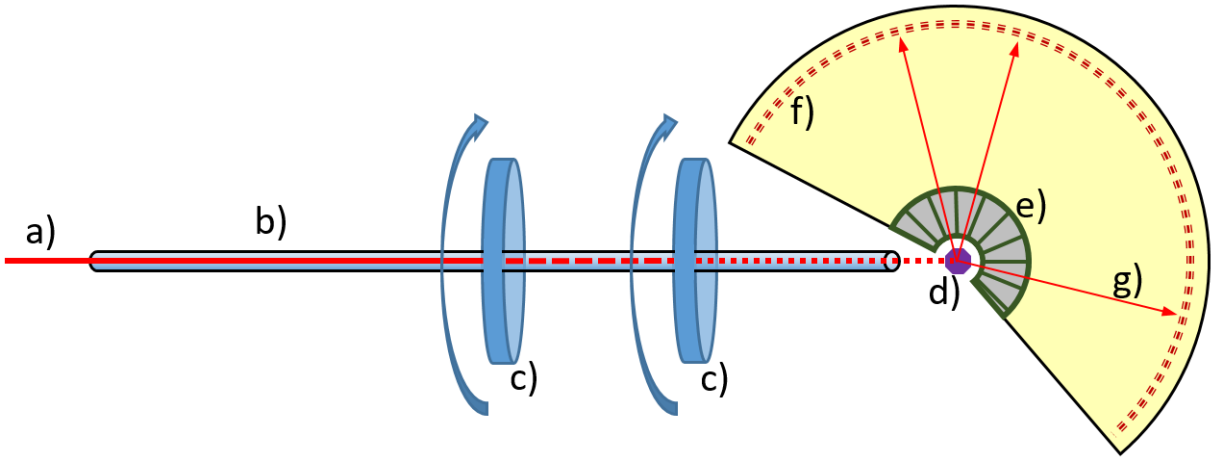

Figure 1. Schematic sketch of the TOFTOF instrument (FRM II, Garching) with a) incident neutron beam, b) neutron guide, c) chopper system, consisting of 7 rotating chopper discs, d) sample position, e) radial collimator, f) detector bank and g) exemplary flight paths of scattered neutrons.

In total, seven chopper discs cut short monochromatic neutron pulses out of the initially white, continuous beam and provides a sufficient distance between and “shortness” of the pulses to avoid frame overlap and ensure good resolution. These short, monochromatic pulses are scattered at the sample. Scattered neutrons are detected in four-meter distance from the sample and their energy transfer with the sample can be calculated from their time-of-flight. From this energy transfer and the scattering angle, one can gain information about dynamic processes in the sample.

TOFTOF has been intensively applied to study polymer and solvent dynamics, mainly in solutions.[2,3,4,5] In recent time, this has been extended towards the investigation of solid films. These films are dropcast from solution and are between 10 µm and 50 µm thick to ensure sufficient scattering statistics. Currently, we are performing QENS experiments on the system PTB7:PCBM. Therefore, we investigate films of pure compounds as well as different blends, which are assumed to form bulk heterojunction structures during fabrication. These BHJ

structures, as sketched in *Figure 2*, are desirable for photovoltaic application due to their morphology on nm-length scale.

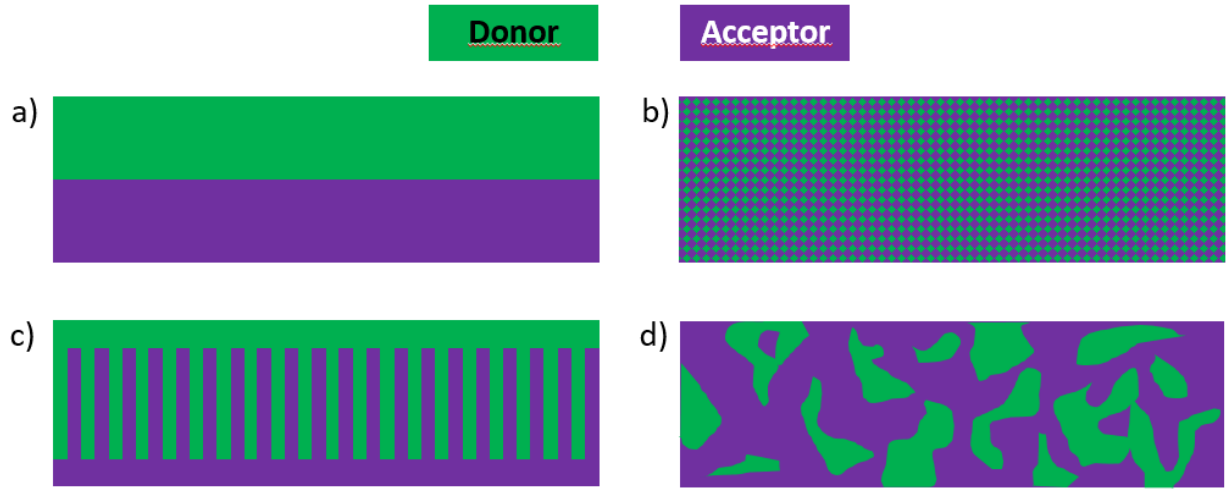

Figure 2. Schematic morphologies of bulk heterojunction thin film cross-sections. a) two layer device; b) very fine, pseudo-homogeneous mixture; c) perfect morphology, as desired for solar cell application, large interface, no short circuits; d) typical BHJ-structure as obtained by solution processing techniques

It is well known that changes in temperature have considerable influence on electric properties of materials and thus on the performance of solar cell devices. Our research goal is to determine dynamic properties of BHJ structures, as shown above, in dependence of temperature and material composition.

An exemplary stack of recorded spectra is displayed in *Figure 3*. It shows the energy transfer for a sample that contains a 1:1 wt. ratio blend of PTB7 and PCBM at a Q-value of 1.05 $Å^{-1}$ at temperatures between 200 K and 400 K.

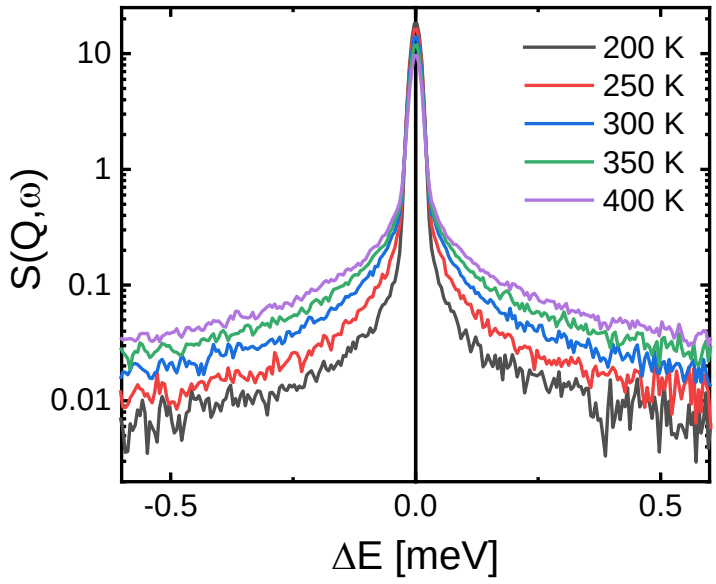

Figure 3. QENS spectra of the blend PTB7:PCBM (wt. 1:1) for temperatures between 200 K (black curve) and 400 K (violet curve). Data were recorded at an average Q-value of 1.05 $Å^{-1}$.

Figure 3 shows that curves, taken at higher temperatures, are broader around the central elastic peak. This indicates an increased energy exchange between atoms/molecules in the sample and the neutrons, which are scattered inelastically, or as called here: quasielastically. By applying particular models, we can draw conclusions about vibrational and diffusional processes inside the respective BHJ material. These processes do influence the electrical properties of the material and are therefore directly linked to device performance. We investigate how blending, as well as the use of alternative materials and additives, influences the molecular dynamics and try to correlate our findings with performance and structural data.

References

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