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Dynamics in polymer-fullerene blends and the influence of DIO as solvent additive studied with quasielastic neutron scattering

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In the emerging field of organic photovoltaics, donor - acceptor bulk heterojunctions are often used as active materials due to their superior performance compared to e.g. planar layered devices. In this optically active polymer layer, photons are absorbed and free charges are created.

A frequently applied and well-studied system is the combination of PTB7 as electron donor and PCBM as electron acceptor. Besides a large number of studies on structure and electrical properties, the level of knowledge about dynamics in this system is very limited, even though molecular mobility plays a vital role in e.g. film formation and degradation processes. We investigated blend films of PTB7 and PCBM, prepared from chlorobenzene solution. The use of solvent additives such as DIO in the production process can significantly increase the power conversion efficiencies of resulting devices but also brings additional challenges in terms of stability. Quasielastic neutron scattering experiments at the cold neutron time-of-flight spectrometer TOFTOF (MLZ, Garching) were performed to determine hydrogen dynamics on a pico- to nanosecond timescale in both, pure PTB7:PCBM blend films and their variation, produced with DIO as solvent additive. The results indicate the presence of residual solvent in the latter samples, however, time resolved measurements during heat treatment reveal different kinetic behavior for solvent removal and the underlying 'aging' of the polymer dynamics.

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