Sub Area 3-2: Organic and inorganic thin-film photovoltaics, III-V high-efficiency devices and related technologies.

Modelling the dynamics of charge extraction transients from organic photovoltaic devices using generative representation learning

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The time-resolved charge extraction (TRCE) technique is used to measure photogenerated charge carrier density (n) within organic photovoltaics (OPV) devices, thereby, enabling characterisation of carrier generation yield and recombination lifetime.[1] Typical analysis of measured TRCE transients (extracted charge over time, see Figure 1) involves simple integration to obtain n. However, each measurement contains a wealth of additional information that is currently not utilised.

The extraction dynamics (and therefore transient shape) are a complex result of the initial spatial and energetic distribution of charge carriers within the device, and their subsequent transport (drift and diffusion) to the device contacts for extraction. Through controlled modulation of the measurement conditions (such as initial excitation density, applied extraction bias, and excitation-extraction delay time) a detailed characterisation of the OPV system's behaviour is obtained. Figure 1 presents example transient sets, illustrating this complexity of extraction dynamics. Further transient analysis can enable the study of respective charge carrier mobilities and recombination lifetimes as a function of n and occupancy within the trap state density distribution.

We have developed a 'model-free' approach for the modelling of TRCE transient datasets, employing generative representation learning methods to implicitly capture the system dynamics, and provide a dissentangled latent-state space representation of the underlying physical mechanisms for investigation.[2] Applying this combination of learned dynamics model and latent-state representation enables the study of OPV system parameters including n-dependent carrier mobilities, recombination lifetimes, and density of states distribution. Additionally, this allows a direct comparison between equivalent measurements of different OPV material systems and device architectures. As such, this analysis greatly enhances the existing capability and usefulness of the TRCE technique, enabling greater detail of characterisation and understanding of next-generation photovoltaic technologies including perovskites and tandem solar cells.

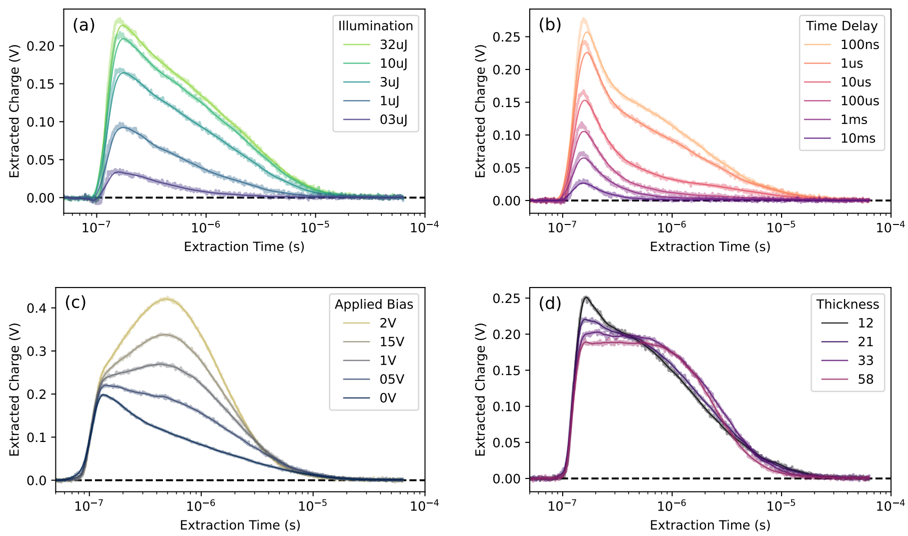

Figure 1: Example charge extraction transients as a function of: (a) laser illumination intensity, (b) excitation-extraction time delay, (c) applied extraction bias, and (d) device active layer thickness; illustrative of the complex dynamics involved.

[1] B. Wright *et al*, Adv. Energy Mater., 2017, 7, 1602026; [2] B. Wright *et al*, AIP Conf Proc, 2022, [*pre-print*]