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Molecular Dynamics Supported In Situ X-Ray Scattering on Organic Solar Cell Layers

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Motivation
Organic solar cells are presently only used for niche applications due to their semi-transparency, flexibility, low weight, and possibilities of custom designs in terms of colours and shapes, but with their low-cost solution processing and projected energy payback times of only fractions of those of silicon modules, the technology has a great potential to reach commercial viability within few years. However, upscaling the fabrication of organic photovoltaics (OPVs) from laboratory-scale devices to large-scale modules without compromising the device efficiency demands an understanding of the microstructure formation during post-deposition drying of the active layer. By combining the strengths of molecular dynamics (MD) modelling and in situ X-ray scattering, we aim to identify the processing parameters that are key to overcome this lab-to-fab challenge and move towards cheap, large-scale, and non-toxic solar cells with record efficiencies.

Simulating post-deposition drying
The efficiency of solution processed OPVs is crucially dependent on the 3D mesoscale thin-film morphology, which in turn is greatly influenced by solvent properties and evaporation rate. In order to reliably simulate active layer morphologies from MD simulations, we have scripted a range of evaporation schemes incorporating e.g. potential walls mimicking substrate—air interfaces as well as including a suspended solvent vapour above the film from which solvent molecules are continuously removed.1

Approaching experimental time-scales
Using the MARTINI force field6 to coarse-grain our systems, the time- and length-scales relevant for morphology evolution are within reach of MD simulations.3,4

Overcoming the lab-to-fab challenge
The knowledge gained from these studies can be used to pin-point the optimal processing conditions for large-scale fabrication of organic solar cells.

References
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6 W. L. Jorgensen et al., Yale University, Department of Chemistry.