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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– and air interfaces as well as including a suspended solvent vapour above the film from which solvent molecules are continuously removed.[1]
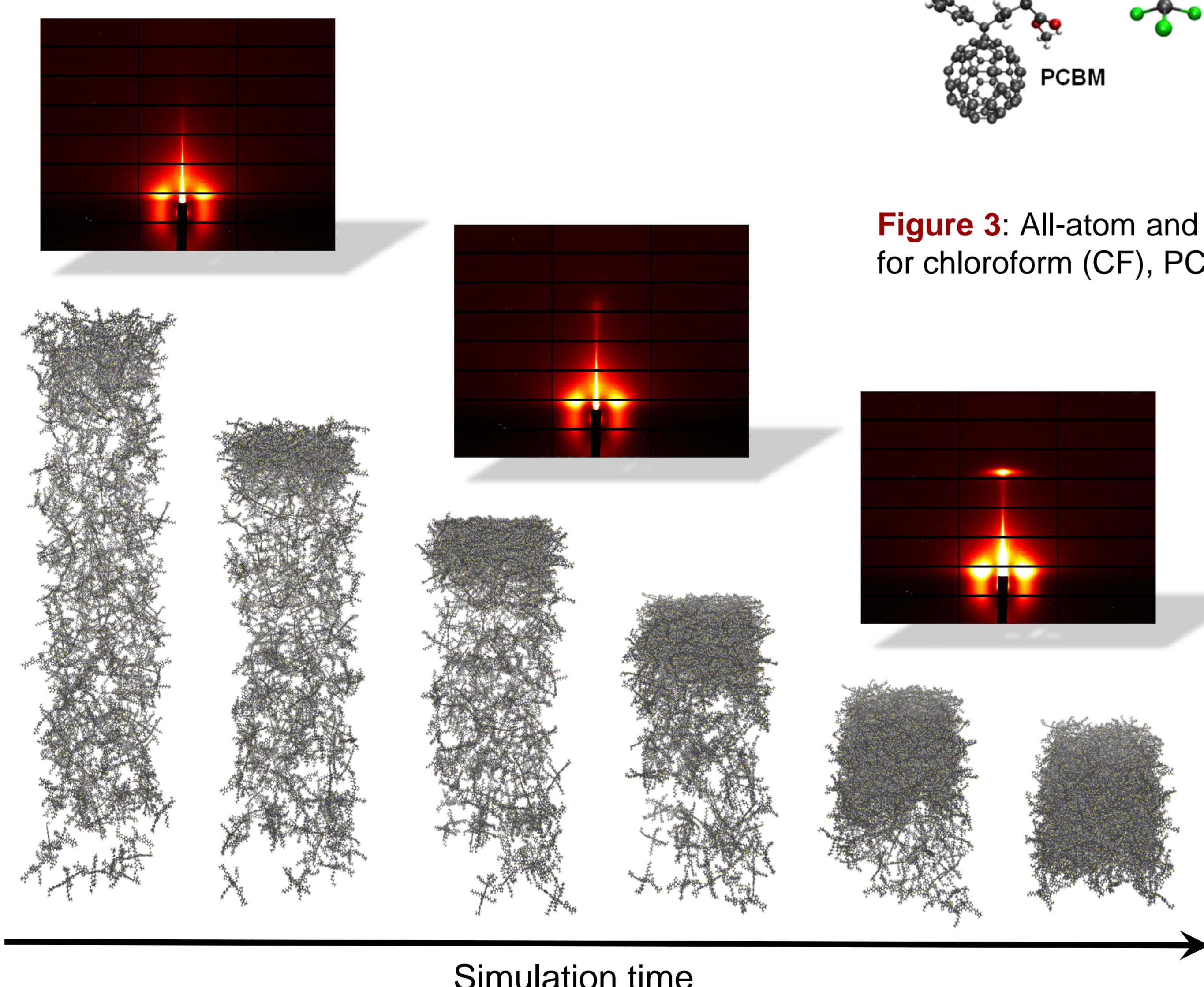
Approaching experimental time-scales

Using the MARTINI force field[2] to coarse-grain our systems, the time- and length-scales relevant for morphology evolution are within reach of MD simulations:[3,4]
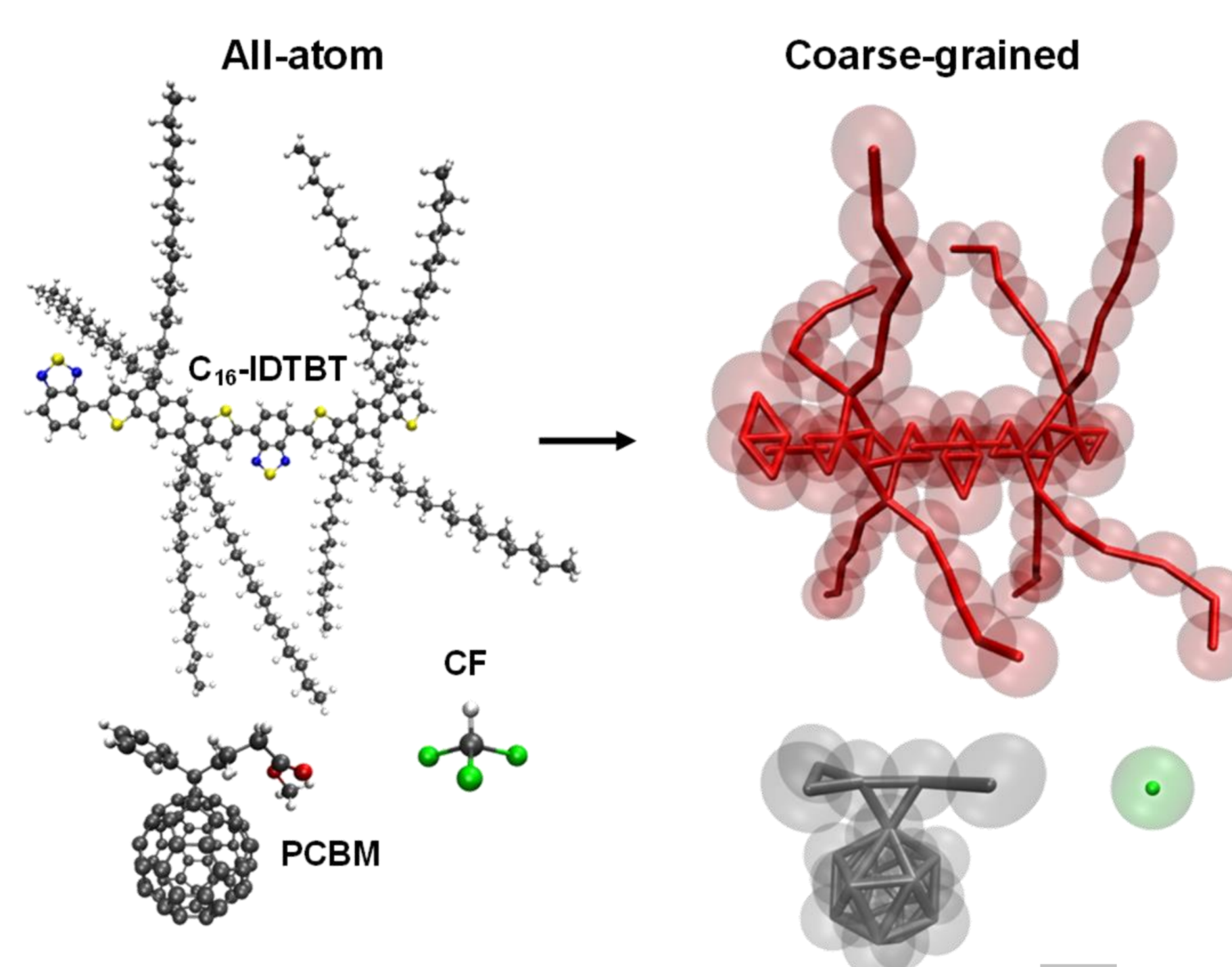

Figure 3: All-atom and MARTINI coarse-grained models for chloroform (CF), PCBM,[4] and a dimer of C_{16}-IDTBT.

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.
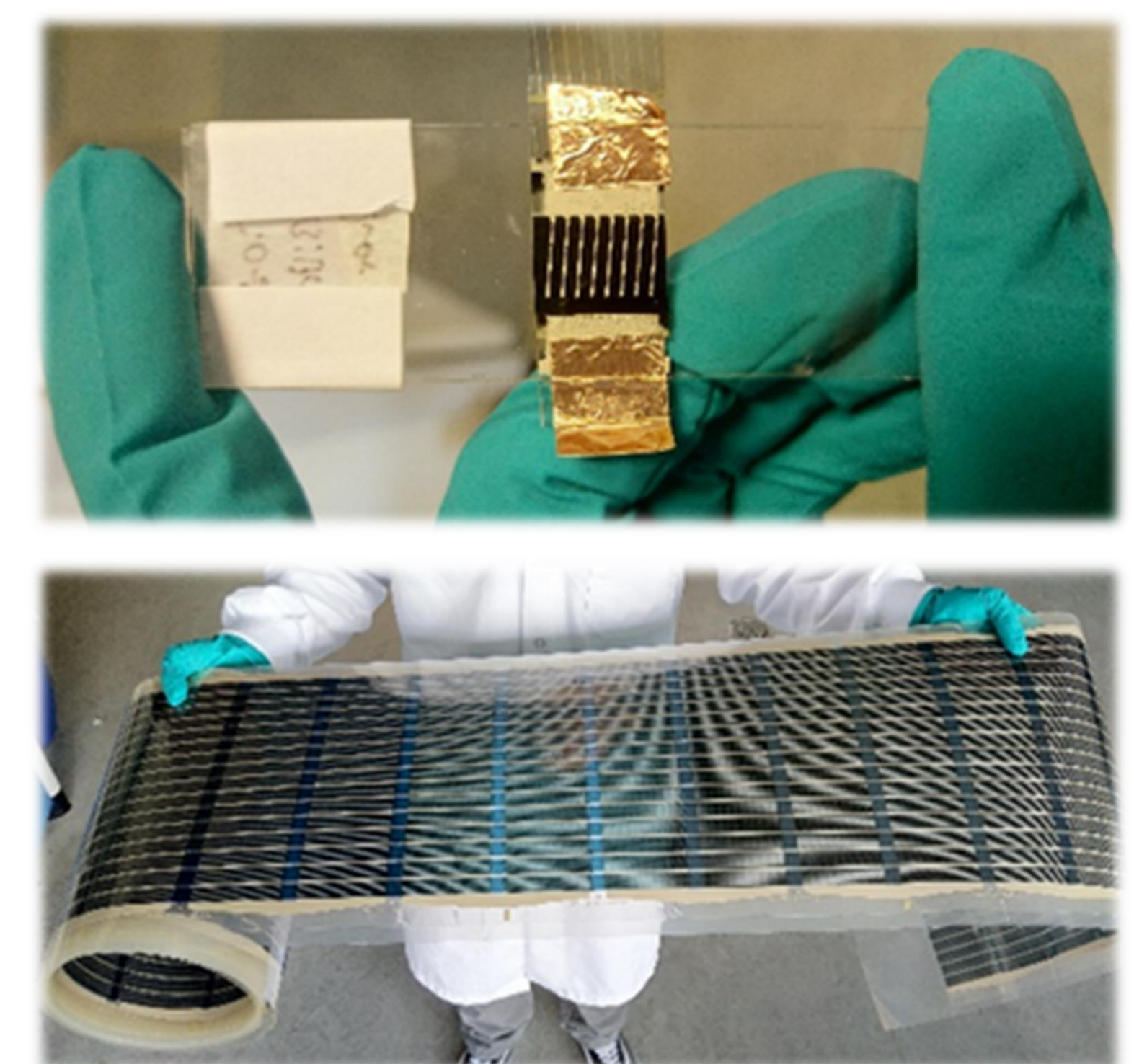

Figure 4: Scalably deposited, flexible OPVs (A. S. Gertsen *et al.,* in peer review, Energy Environ. Sci.).

L A B to F A B

Simulation time

Figure 1: Solvent evaporation simulation and examples of corresponding grazing incidence small-angle X-ray scattering (GISAXS) signals recorded at cSAXS, SLS.
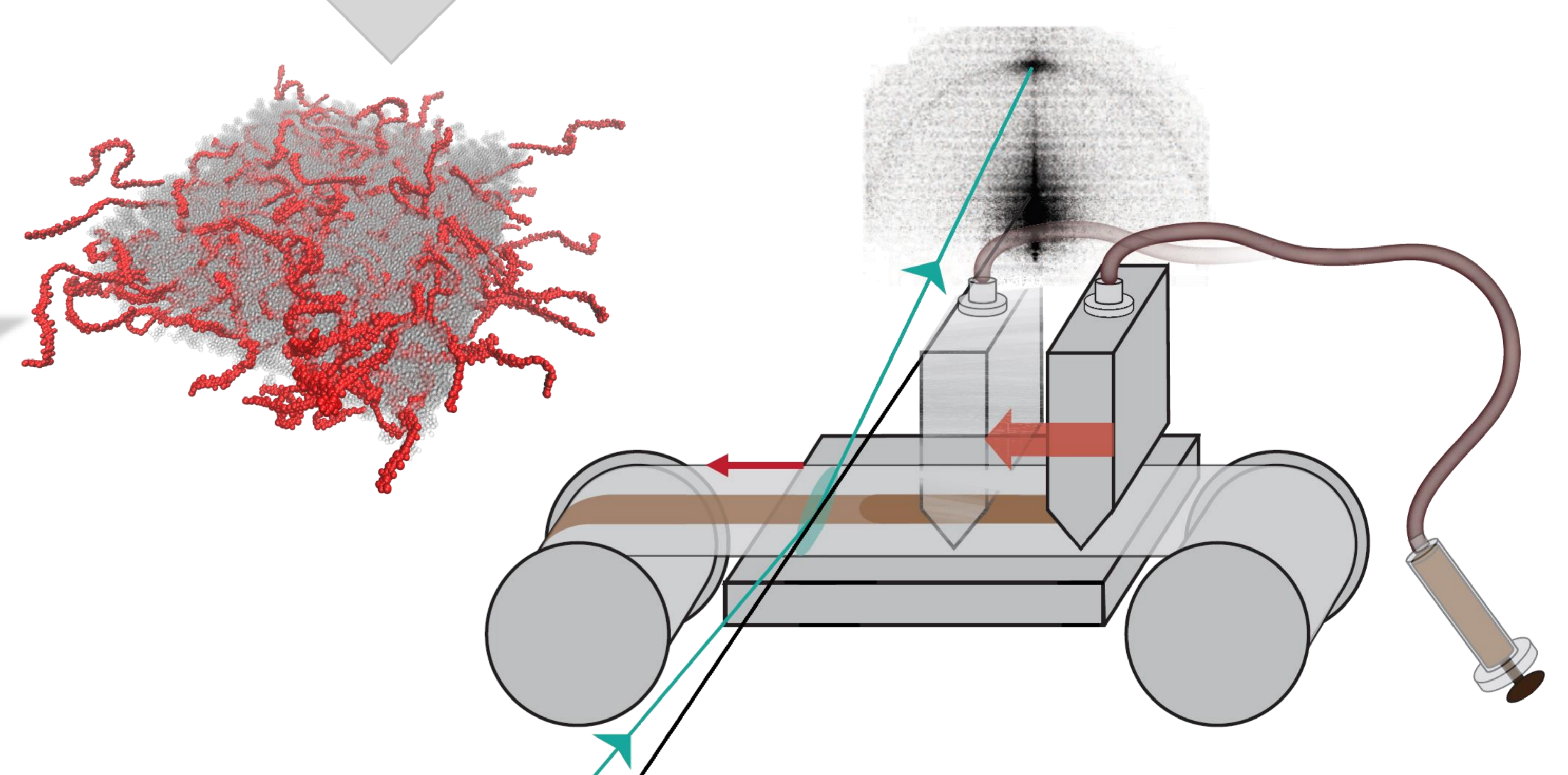

Figure 2: Schematic of the roll-to-roll slot-die coating setup used for *in situ* GISAXS experiments at the cSAXS beamline, SLS (adapted from Ref. 5).

Methodology

We have used the GROMACS 2016.3 package for all MD simulations. The OPLS-AA force field[6] formed the basis for the all atom simulations with our own parameterizations of e.g. most angles and in particular the inter-monomer torsional potentials and sidechain couplings – these were based on quantum chemical DFT calculations. The coarse-grained simulations were based on the MARTINI force field[2] and in part Ref. 4.

References

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