Abstract Submitted
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Kinetic Monte Carlo simulation of organic devices ALISON WALKER, EDWARD WRIGHT, University of Bath — At Bath, we have developed a model of organic devices that links morphology (packing arrangements) to device characteristics. The model, based on the dynamical Monte Carlo approach pioneered in surface physics, allows us to include interaction processes between different species on many different timescales. In this talk I will show how we have used this approach to compare organic solar cells of rod, blend and gyroid morphologies and to model the influence of interlayers, layers added to improve efficiency and lifetime, in organic light emitting devices, OLEDs. We have developed the model to allow it to distinguish between triplet and singlet excitons and allows for the interactions of these species (triplet-triplet annihilation, triplet-singlet annihilation, triplet-polaron quenching). I will show our predictions for current-voltage-illumination characteristics (solar cells) and current-voltage-luminance characteristics (OLEDs). I will also show how through prediction of emission zone profiles in an OLED, we can gain insight into what determines changes in OLED efficiency with current and how in the longer term this approach can be used to address degradation.

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