Kinetic Monte-Carlo techniques for modeling and simulation or organic semiconductors

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A multi-particle 3-dimensional Kinetic Monte Carlo, KMC, model has been developed to model the link between morphology and device performance at the mesoscopic level. This model adopts a random walk hopping approach that **includes interactions between particles on many different length and timescales in complex materials packing arrangements**. We have used this approach to show how balanced charge transport can be improved in organic light emitting devices, OLEDs [1]. In organic photovoltaics (OPV) we have looked at how geminate and bimolecular electron-hole recombination reduce device performance and explained measuired device characteristics in planar and blend devices [2].

The approach we use, the First Reaction Method [3], is dynamically correct, meaning that a proper temporal sequence of events is maintained. I will demonstrate how it can be applied to a wide variety of electrical and energy transport problems such as recombination in OPV[4], doping in dye-sensitized and perovskite cells [5] and the influence of triplet and singlet exciton dynamics on luminosity, current density and luminous efficiency of OLEDs with and without an interlayer in a comparison with measured data[6].

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References

[1] J Bailey, E N Wright, X Wang, A B Walker, D D C Bradley,J-S Kim *J Appl Phys* (2014) **115**, 204508
[2] R G E Kimber, E N Wright, S E J O'Kane, A B Walker, J C Blakesley *Phys. Rev. B* (2012) **86**, 235206
[3] J J Lukkien, J P L Segers, P A J Hilbers, R J Gelten, A P J Jansen *Phys. Rev. E* (1998), **58** 2598.
[4] C Groves, R G E Kimber, A B Walker, *J. Chem. Phys.* (2010) **133** , 144110
[5] A Abate, D R Staff, D J Hollmann, H J Snaith, A B Walker*Phys. Chem. Chem. Phys.* **16** , 1132 (2014)
[6] M. Roberts et al *Proc. SPIE 7722, Organic Photonics IV* **7722** (2010), 772201 (Eds P. L. Heremans, R, Coehoorn, C. Adachi)