**Mesoscale simulations of polymer based organic photovoltaics, OPV**

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Alignment to aims of PV-CDT. OPV efficiencies must be improved if they are to compete with perovskite solar cells. This proposal will probe a means of establishing molecular design strategies for OPV materials that is particularly directed at polymers. It is of interest to CDT partners working in OPV and an Australian group. Merck have indicated informally that they are interested in funding 50% of a studentship. Transferable skills training comes from University of Bath and online courses on parallel techniques and software engineering.

Project description While the focus on energy level tuning in OPV materials has afforded large gains in device performance, strategies based on morphol-ogical control are at least as promising[[1]](#footnote-1). A mesoscopic model of charge transport in polymers should explicitly allow for long chains as illustrated in Figure 1[[2]](#footnote-2). The link between efficiency and morphol-ogy in cells that include polymers is accentuated by differences between intra- and inter-chain charge transportt[[3]](#footnote-3). Intra-chain transport is often faster, for example in ‘disorder free’ polymers[[4]](#footnote-4).   
 The Framework Rigidity Optimized Dynamic Algorithm, FRODA, based on constrained molecular dynamics, MD, has been used in protein simulations[[5]](#footnote-5). With a Supersolar Hub studentship cofunded by Merck 2013-17, we have shown FRODA can be adapted to predict morphologies for conjugated small molecules and polymers including fullerenes. FRODA has the significant advantage that it avoids the need for coarse graining, CG[[6]](#footnote-6), by focussing on the modes with low phonon frequencies responsible for packing. A direct link between chemical structure and morphology has been established for system sizes ~104 atoms in a cell ~ 10 nm in a workstation with a graphics card similar to those used for gaming machines. Tailored software has been developed for visualising the atomic structure during the simulation. Kinetic Monte Carlo, KMC, calculations of charge mobilities for charge hops between conjugated segments2 on FRODA morphologies will be compared with measurements on Organic Field Effect Transistors, OFETs made at Merck.   
 In this project, FRODA will be modified to look at morphologies that contain electron donors and acceptors (year 1). In years 2-4, the KMC code employing FRODA will be combined with the Bath OPV codes for lattice KMC[[7]](#footnote-7) that allow for multiple species (electrons, holes, singlet and triplet excitons). System sizes will be increased to ~107 atoms in a cell ~100 nm by parallelising the geometric simulation engine in FRODA, for use on High Performance computers. Links with the experimental groups of Dr Da Como and others will be used for code validation and exploitation. Dr K Feron, CSIRO Newcastle Australia, is interested in using this approach to study OPVs that include core shell nanoparticles[[8]](#footnote-8) and we are looking at ways for joint funding of graduate student exchanges. Codes will be made open source where possible given constraints due to the potential industrial interest and the use of FRODA.

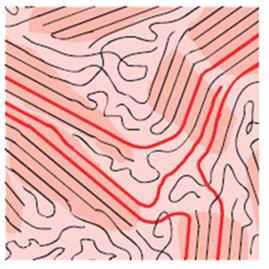


Fig. 1 Schematic diagram of morphology of a polymer film; long chains are highlighted in red

1. N E Jackson et al J Phys Chem Lett Just accepted (2014) [↑](#footnote-ref-1)
2. R Noriega et al Nature Materials (2013) **12** 1038 [↑](#footnote-ref-2)
3. A Van Vooren et al ChemPhysChem (2008) **9**, 989 and Y Olivier et al Adv Mat (2014) **26** 2119 [↑](#footnote-ref-3)
4. D Venkateshvaran et al Nature (2014) **515** 384 [↑](#footnote-ref-4)
5. S Wells et al Phys. Biol. (2005) **2** S127 [↑](#footnote-ref-5)
6. D M Huang, A J Moule, R Faller Fluid Phase Equilibria (2011) **302**, 21 [↑](#footnote-ref-6)
7. R G E Kimber et al Phys. Rev. B (2012) **86**, 235206 [↑](#footnote-ref-7)
8. K Feron et al J Appl Phys (2014) **116**, 124502 [↑](#footnote-ref-8)