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### **Multiscale modelling of charge transport in organic electronic materials**

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Charge transport in disordered organic semiconductors is controlled by a complex combination of phenomena that span a range of length and time scales. As a result, it is difficult to rationalize charge transport properties in terms of material parameters. Until now, efforts to improve charge mobilities in molecular semiconductors have proceeded largely by trial and error rather than through systematic design. However, recent developments have enabled the first predictive simulation studies of charge transport in disordered organic semiconductors. In this presentation we will show how a set of computational methods, namely molecular modelling methods to simulate molecular packing, quantum chemical calculations of charge transfer rates, and Monte Carlo simulations of charge transport can be used to reproduce experimental charge mobilities with few or no fitting parameters. Using case studies, we will show how such simulations can explain the relative values of electron and hole mobility and the effects of grain size, side chains and polymer molecular weight on charge mobility. Although currently applied to material systems of relatively high symmetry or well defined structure, this approach can be developed to address more complex systems such as multicomponent solids and conjugated polymers.