Charge and exciton transport are well understood in two extremes: in highly ordered materials, transport is by band conduction, while in highly disordered ones, it is by hopping. In moderately disordered materials, the approximations valid in either extreme break down, making it difficult to accurately model the conduction process. Materials where this may be an issue include organic semiconductors, metal organic frameworks, hybrid perovskites, and quantum dots. In particular, charges and excitons in organic semiconductors are usually assumed to be localised onto individual molecules (or segments of polymers), but intermolecular couplings mean that there is usually some (partial) delocalisation across multiple molecules. Theoretically describing the movement of partially delocalised carriers is difficult, because it depends on a complicated interplay of energetic disorder, quantum-mechanical couplings, and polaron formation.

We report a new method that is able to describe the motion of partially delocalised charges and excitons in all regimes of disorder. We also implement numerical innovations to allow us to work in three dimensions, a regime that had proven too complicated for all comparable approaches. Our results reveal new, basic physics of transport in organic semiconductors, explain why mobilities predicted by traditional kinetic Monte Carlo are usually too low, and show how three-dimensional calculations capture effects missing in lower-dimensional approximations. We also discuss extending our method to describe charge separation, an effectively six-dimensional process in which delocalisation is suspected to play a critical role.

Time: Wednesday 17th July, 9:00-10:00
Location: PNS seminar room no. 5.1.00.001, Building PNS, ground floor