Electric Field Control of Quasiparticle Wavefunctions in Organic Semiconductors

UCL Lead department: Physics & Astronomy

Lead Supervisor: Prof Jochen Blumberger

Project Summary:

Background: Being able to control the electronic state of quasiparticles (excess electrons, electron holes, spins, excitons,…) in condensed phase materials is a dream-goal and would upon up myriad novel applications in energy conversion and quantum technology. Ordered organic semiconductors provide an attractive materials platform in this respect where quasiparticles form localized waves and move in a shallow energy landscape that can be easily modified by relatively weak external electric fields. For instance, our group has shown that an electron hole injected in a rubrene crystal is delocalized over about 13 molecules after thermalisation at room temperature and diffuses about one lattice spacing (~1 nanometer) every 100 femtoseconds due to thermal excitations of the hole in the valence band in what we called transient delocalization mechanism[1,2]. **In this project we aim to demonstrate that it is possible to exert precise control over the time evolution of quasiparticle wavefunctions in organic semiconductors, specifically their location in the crystal lattice and the extent of delocalization, using Terahertz (THz) electric fields.**

Contribution: In the project you will extend a novel quantum dynamical simulation methodology that our group has developed[1] by implementing the interaction of quasiparticles with static and oscillating electric fields. You will carry out simulations to explore if the mean position of the wavefunction can be pinned to/trapped at a specific location in the lattice by applying an electric field with a frequency comparable with the free diffusive motion between lattice sites, 1-10 THz. Then you will investigate how wavefunction delocalization can be controlled by varying field strength. Finally, using control theory you will design THz electric field sequences (e.g.,pulses) to move the quasiparticle wavefunction to any arbitrary location within the material.

Impact: This work will provide a proof of concept how the time evolution of a quasiparticle in OS can be controlled in space and time using external electric fields. I anticipate that our predictions can be realised by pump-THz probe spectroscopy experiments similar to the ones used to probe charge mobility. In the long term, our ability to control the nature of quasiparticles in OS materials is expected to open up new horizons in energy science and quantum technology.

Highly motivated students from Physics, Chemistry or Materials Science Departments are strongly encouraged to apply for this post. Good knowledge in quantum mechanics and statistical mechanics and interest in writing computer code is expected. Some experience with molecular simulation and scripting languages (e.g., Python) is a plus. Informal enquiries regarding the vacancy can be made to Jochen Blumberger, j.blumberger@ucl.ac.uk.

[1] S. Giannini et al. *Nat. Commun.* 10, 3843 (2019).

[2] S. Giannini et al. *Nat. Mater.* 22, 1361 (2023).