



**NECEM SEMINAR: "Modelling of organic semiconductors for solar energy harvesting, data storage and sensors - from molecules to devices"**

**Dr. Roderick MacKenzie**

**From the University of Nottingham, UK**

**Wednesday 30<sup>th</sup> October 2019, 2-3pm**

**Durham University, E240, Engineering Higginson Building 2-3**

**Refreshments available after the seminar**

Modelling of organic semiconductors for solar energy harvesting, data storage and sensors - from molecules to devices

Over the last 20 years there has been an intense search to find alternatives to traditional inorganic semiconductors such as Silicon and Gallium arsenide, which are used in the current generation of solar cells, light emitting diodes, and sensors. To produce efficient devices, the materials from which they are made must be highly pure (>99.9999%), and achieving this purity requires significant energy expenditure during manufacture, resulting in significant CO<sub>2</sub> generation, a high system cost and a long energy pay back times. Organic semiconductors based on conducting plastics and small molecules offer a more environmentally friendly replacement to Silicon, as they require significantly lower energy input to manufacture. In this talk, I will introduce the fundamental physics of charge transport in disordered organic semiconductors, and explain how this understanding can be used to design better optoelectronic devices made from these novel materials. The talk will cover charge transport on the microscopic level, addressing how charge is generated, transported and recombines in these conducting plastics. The talk will then discuss the development of macroscopic drift-diffusion models simulate whole devices made of these highly disordered organic materials from the steady state [1,2] to the femtosecond time scale [2]. At the end of the talk we will discuss the application of new machine learning based techniques to accelerate some of these modelling approaches.

[1] W. R. Erwin, et al. "Understanding the Limits of Plasmonic Enhancement in Organic Photovoltaics", The Journal of Physical Chemistry C 122, 7859-7866, 2018

[2] H. Mäkel and R. C. I. MacKenzie "Determination of Charge Carrier Mobility in Disordered Thin-Film Solar Cells as a Function of Current Density", Physical Review Applied, 9, 034020, 2018

[3] R. C. I. MacKenzie, et al. "Theory of Stark spectroscopy transients from thin film organic semiconducting devices", Physical Review B 89, 195307, 2018



## Location

Durham University, E240, Engineering Higginson Building 2-3

(<https://www.dur.ac.uk/map/> engineering pin on this link)

