ISSC-24 talk – Alan Bowman

Title: Combining photoluminescence and first principals modelling to probe the nanoscale

Light driven machines, including solar cells, photochemical and photoelectrochemical devices, are being rapidly developed as we transition towards a zero carbon society. Interfaces play a key role in all these devices. They must be optimised in order to achieve high efficiencies, requiring a combination of state-of-the-art measurement techniques and modelling. In this talk I present two examples of the power of combining photoluminescence and first principals modelling.

Enabling efficient triplet charge transfer between singlet fission materials and halide perovskite semiconductors is key to realising a new form of highly efficient solar panel. Here we used photoluminescence to observe this charge transfer. Our results motivated us to simulate two-particle excited states at this interface, which revealed bottlenecks for charge transfer and identified new routes to better control the interface.

Nanoscale plasmonic metals represent a route to catalysing chemical reactions. However, probing electronic processes non-invasively is extremely difficult at such small length scales. In the second part of this talk I will discuss our recent efforts to understand photoluminescence from nanoscale, atomically flat, gold films via density functional theory (DFT). I present a model of photoluminescence which explains our observations and paves the way to a new probe of chemical reactions at nanometer length scales.

These works showcase the potential of combining spectroscopy and DFT within a single study, and, excitingly, at comparable length scales. Ultimately this enables new approaches to optimise sustainability related devices.