



NECEM WEBINAR: Multi scale modelling of organic devices and perovskite solar cells

Prof Alison Walker

University of Bath

Wednesday 22nd April, 2-3pm

Zoom: <https://newcastleuniversity.zoom.us/j/99405152728>

All welcome

Multi scale modelling of organic devices and perovskite solar cells

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I will describe my group's research on organic electronics and perovskite solar cells and light emitting diodes, LEDs. Our aim is to develop realistic models that efficiently connect phenomena at different length-scales synergistically with experiments to quantitatively predict device performance. These models focus on different scales of resolution, atomistic scale through mesoscale to continuum (macroscale). Combining the models allows us to understand how microscopic processes governing charge and energy transport influence behaviour, e.g. charge mobilities.

For organic devices, I will describe our use of kinetic Monte Carlo models at the mesoscopic level. I will describe simulation of charge and energy transport in small molecule and polymer semiconductors with a recently developed fast electrostatics solver and with morphologies obtained with the code Simulation of Atomistic Molecular Structures using an Elastic Network (SAMSEN) developed by my group [1]. Large systems, e.g. 100 polymers each 10 monomers long, can be simulated with SAMSEN in around a day with a desktop computer.

In perovskite solar cells and LEDs, I will describe how our drift diffusion model of ionic-electronic conduction has shown how mobile ion vacancies cause hysteresis. I will also demonstrate predictions from a mesoscopic model in which the charge carriers are treated as polarons and that shows the conditions under which hot polarons can beat the Shockley-Queisser limit.

References

[1] A R Smith, I R Thompson, A B Walker J. Chem. Phys. 150, 164115 (2019)



Engineering and
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Biography



Alison Walker was born in Sarawak on the island of Borneo. Her undergraduate and postgraduate degrees were at the University of Oxford, followed by postdocs at Michigan State University USA and at Daresbury. She took up a lectureship at the University of East Anglia, moving to the University of Bath in 1998. A Royal Society Industry Fellowship with Cambridge Display Technology led to her coordinating 4 EU projects, including training networks, along with coleading the Centre for Doctoral Training in New and Sustainable Photovoltaics. She is a member of the physics assessment sub panel for REF21 and chairs the Solar

Commission aimed at publicising the role of solar in the UK economy.