NECEM WEBINAR:
"Opportunities and challenges in solution-processable inorganic thin-film photovoltaics"

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Via Zoom email: justina.heslop@newcastle.ac.uk for access.

In this webinar, I will be presenting some of our past work done during my tenure at the University of Bristol.

Future sustainable thin-film solar cell (TFSC) technology for utility-scale, as well as building-integrated applications, requires the development of green and low-cost alternative absorbers to existing $Cu(In,Ga)Se_2$ and CdTe. Cu_2ZnSnS_4 (CZTS, Kesterite) structurally and electronically similar to $Cu(In,Ga)Se_2$ is a potential candidate for stable all inorganic device configuration composing earth-abundant, low-cost and non-elements. Despite considerable efforts, the best lab-scale device efficiency (~ 13%) remains below the performance level needed to meet the balance-of-systems costs. The challenge could be overcome by (i) further lowering the solar fabrication costs with employing low-cost solution methodology instead of conventional vacuum techniques and (ii) improving device performance by understanding and resolving the bulk as well as interfacial recombination pathways. This presentation would exhibit our rational methodology to address both these issues.

First, I will describe our approach to fabricate high-quality kesterite thin films and to introduce Sb and Na doping to improve device performance[1–4]. This is being supported by extensive material characterization based on XRD, Raman spectroscopy, electron microscopy, XPS and diffuse reflectance spectroscopy shows the formation of phase pure crystalline kesterite thin films with an optical band gap of 1.4 eV. Devices with the architecture glass/Mo/kesterite/CdS/i-ZnO/ZnO:Al/Ni-Al are constructed and investigated on sub-module dimensions (5x5 cm^2) platforms[1,3].

In the second part, I will elaborate on our efforts to correlating structural, optical and electronic signatures of defects in the active layers which are detrimental to cell performance[3]. Our approach includes a unique combination of variable temperature dependent impedance and photoluminescence spectroscopy, as well as energy-filtered photoemission microscopy[5]. Contrary to models proposed in the field, attributing performance losses to Cu-Zn antisite disorder, we demonstrate that Sn disorder is critical in voltage losses and how Sb and Na doping can selectively remediate these defects.

In the last part of the presentation, I will briefly showcase some of the recent work and my current interest on the emerging class of 'defect-tolerant' semiconductors through the examples of BiI_3[6], BiSI[7], $BiPS_4$[8]. In a nutshell, with over 4000 test devices,[1-11] some of which pioneering and delivering record efficiencies, the versatility of our synthetic methodology will be demonstrated.

***** The presented work was performed in collaboration and is co-authored with:

- *University of Bristol*: Prof. David Fermin, Prof. Dave Cherns, Dr. Neil Fox, Dr..Mattia Cattelan, Dr. Tom Oliver, Dr. Rob Harniman, Dr. Andrei Sarua, Dr. Dominic Alibhai, Dr. Nessrin Kattan, Ms. Fabiola Cardoso, Ms. Victoria Taylor and Ms. Marta Duchi
- *Helmholtz-Zentrum Berlin:* Dr. Reiner Klenk and Dr. Tristan Koehler
- *University of Strathclyde*: Prof. Rob Martin, Dr. Mike Yakushev and Ms. Ekaterina Skidchenko
- *Rutherford Appleton Lab*: Dr. Paul Donaldson and Dr. Ian P Clark

References: **1.**Tiwari, D. *et al. Chem. Mater.* 28 (2016) 4991–4997; **2.**Tiwari, D. *et al. ACS Appl. Mater. Interfaces* 9 (2017) 2301–2308; **3.**Tiwari, D. *et al. J. Mater. Chem C* 5 (2017) 12720–12727; **4.** Tiwari, D., *Sustain. Energy Fuels* 1 (2017) 899–906; **5.**Tiwari, D. *et al. ACS Energy Lett.* 3 (2018) 2977–2982; **6.** Tiwari, D. *et al. ACS Energy Letters* 3 (2018)1882-1886; **7.** Tiwari, D. *et al. ACS Applied Energy Materials* 2 (2019) 3878-3885; **8.** Tiwari, D. *et al. Chemistry of Materials* 32 (2020) 1235-1242; **9.**Tiwari, D. *et al. J. Phys. Chem C* 119 (2019) 5872-587; **10**. Tiwari, D. *et al. Sustainable Energy & Fuels* 1 (2017) 899-906; **11.** *Taylor, V. et al. J. Phys. Chem Lett.* 9 (2018) 895-901; **12.** Tiwari, D. *et al. ACS applied materials & interfaces 9 (3), 2301-2308*

Biography

I have recently joined Northumbria University as a Vice-Chancellor's Senior Fellow in the Department of Mathematics, Physics and Electrical Engineering. My current research interest lies in understanding the emergence of defect-tolerance in semiconductors and using defect-tolerant semiconductors for PV and solar fuel applications. This involves materials discovery and building structural-activity relationship through a combination of atomistic computational modelling, materials processing and defect-characterization of new inorganic PV semiconductors and devices. I have developed novel methodologies to process complete solar cells using non-vacuum techniques, examining a variety of unconventional absorbers including Cu_2SnS_3, $Cu_2ZnSn(S,Se)_4$, $BiFeO_3$, BiI_3, BiSI, $BiPS_4$. Recently we have been investigating these methodologies to develop PV structures for low-cost system integration (buildings, automotive, etc.) as well. To date, I have published 34 high-quality research articles (google scholar h-index: 16).

My postdoctoral was undertaken at the University of Bristol in Professor David Fermin's lab as a part of an EPSRC project targeting new PV technologies based on solution-processable earth-abundant materials. Before this, I studied chemistry from Sardar Patel University, Gujarat, India (MSc 2009) and completed my PhD in 2014 investigating solution-processed Cu_2SnS_3 thin-films for solar cells at Dr. K. C. Patel research and development centre (CHARUSAT, India). My Doctoral studies were pursued through a UGC-department of atomic energy (DAE) fellowship which involved working part-time at the national facility hosted at the UGC-DAE-Consortium for Scientific Research, Indore, India. My thesis work focused on low-temperature charge-transport measurements and photoemission experiments on semiconductor thin-films and PV devices.