In-situ neutron reflectometry reveals dye: TiO_2 interfacial structures within dye-sensitized solar cell device environments

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The transparent and low-cost nature of dye-sensitised solar cells (DSCs) affords them niche prospects for electricity-generating windows in energy-sustainable buildings. Despite their vast industrial potential, innovation is being held up by a lack of suitable dyes. Better dyes can only be realized if we can better understand how the dye···TiO_2 interface of a DSC working electrode functions at the molecular level. To this end, this talk presents an *in situ* neutron reflectometry study that determines this dye···TiO_2 interfacial structure while housed in its device environment [1]. The high-performance DSC dye, MK-2 and its molecular building block, MK-44 are the case studies [2]. Probing this buried interface within its device environment sets this study apart from surface chemistry approaches that characterize the exposed interfaces. We show how the electrolyte modulates the structure of these buried interfaces, and thence its photovoltaic properties. The finding that this structural modulation is only observed once the DSC working electrode is atomically probed in its device environment highlights the need to characterize these buried interfaces directly, if DSC functionality is to be properly understood at the molecular scale.

References:

[1] J. McCree-Grey, J. M. Cole, S. A. Holt, P. J. Evans, Y. Gong, “Dye···TiO_2 Interfacial Structure of Dye-Sensitised Solar Cell Working Electrodes Buried under a Solution of I^-/I_3^- Redox Electrolyte”, *Nanoscale* (submitted).

[2] J. M. Cole, M. A. Blood-Forsythe, T. C. Lin, P. Pattison, Y. Gong, A. Vazquez-Mayagoitia, P. G. Waddell, L. Zhang, N. Koumura, S. Mori, “Discovery of S···C≡N intramolecular bonding in a thiophenylcyanoacrylate-based dye: realizing charge transfer pathways and dye···TiO_2 anchoring characteristics for dye-sensitized solar cells”, *ACS Appl. Mater. & Interfaces*, submitted.