Electronic Supplementary Information

A comprehensive comparison of dye-sensitized NiO photocathodes for solar energy conversion

Christopher J. Wood,[a,b] Gareth H. Summers,[a,b] Charlotte Clark,[a] Nicolas Kaeffer,[c] Maximilian Braeutigam,[d] Lea Roberta Carbone,[e] Luca D'Amario,[f] Ke Fan,[g] Yoann Farré,[h] Stéphanie Narbey,[i] Frédéric Oswald,[i] Lee A. Stevens,[j] Christopher D. J. Parmenter,[k] Michael W. Fay,[k] Alessandro La Torre,[k] Colin E. Snape,[l] Benjamin Dietzek,[d] Danilo Dini,[e] Leif Hammarström,[f] Yann Pellegrin,[h] Fabrice Odobel,[h] Licheng Sun,[g] Vincent Artero,[c] Elizabeth A. Gibson,[a,b]*

[a] School of Chemistry, The University of Nottingham, University Park, Nottingham, NG7 2RD, UK.

[b] now at the School of Chemistry, Newcastle University, Newcastle upon Tyne, NE1 7RU, UK. Email: Elizabeth.gibson@ncl.ac.uk

[c] Laboratoire de Chimie et Biologie des Métaux, UMR 5249 (CEA-CNRS-Université Grenoble Alpes), CEA-Grenoble, 17 av. des Martyrs, 38000 Grenoble, France.

[d] Institute of Photonic Technology (IPHT) Jena e. V., Albert-Einstein-Straße 9, D-07745 Jena, Germany. Institute for Physical Chemistry and Abbe Center of Photonics, Friedrich-Schiller University Jena, Helmholtzweg 4, D-07743 Jena, Germany.

[e] Department of Chemistry, University of Rome "La Sapienza", Rome, Italy.

[f] Department of Chemistry- Ångström, Uppsala University, Box 259, SE-751 05 Uppsala, Sweden.

[g] School of Chemical Science and Engineering, Royal Institute of Technology (KTH), 100 44 Stockholm, Sweden.

[h] CEISAM, Chimie et Interdisciplinarité, Synthèse, Analyse, Modélisation, CNRS, UMR 6230, Faculté des Sciences et des Techniques Université de Nantes, 2, rue de la Houssinière, BP 92208, 44322 NANTES Cedex 3, France.

[i] Solaronix, rue de l'Ouriette 129, CH-1170 Aubonne, Switzerland.

[j] Division of Materials, Mechanics and Structures, Faculty of Engineering, University of Nottingham, University Park, Nottingham, NG7 2RD, UK

[k] Nottingham Nanotechnology and Nanoscience Centre, University of Nottingham, University Park, Nottingham, NG7 2RD, UK

[l] Department of Chemical and Environmental Engineering, Faculty of Engineering, University of Nottingham, University Park, Nottingham, NG7 2RD, UK

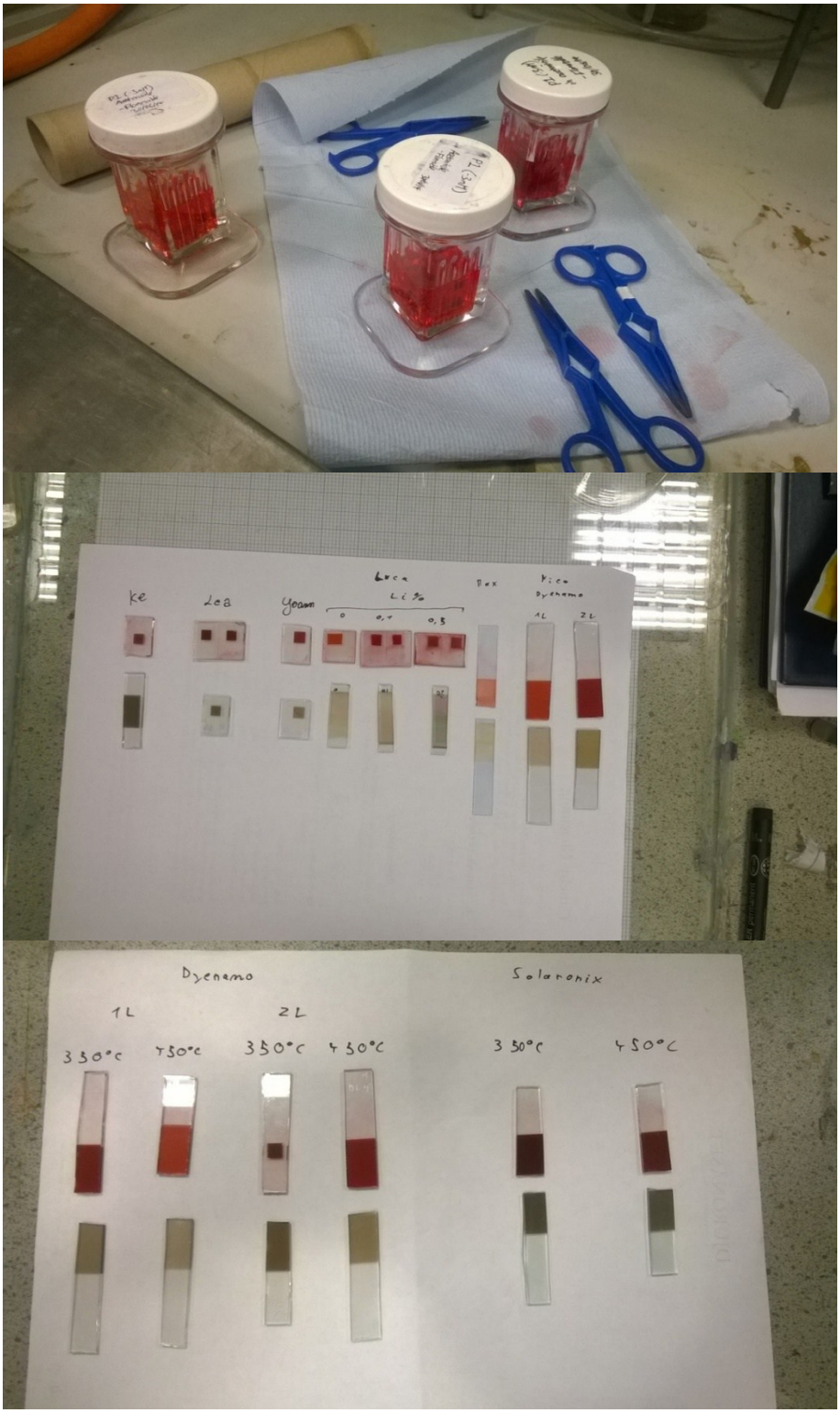

Figure S1. Photos of the samples used in this study. The sensitisation of each sample was identical: (1) Placing of the NiO films in a CH_3CN dye bath containing **P1** 0.3 mM for a period of 16 h. (2) Rinsing of films to remove unadsorbed dye.

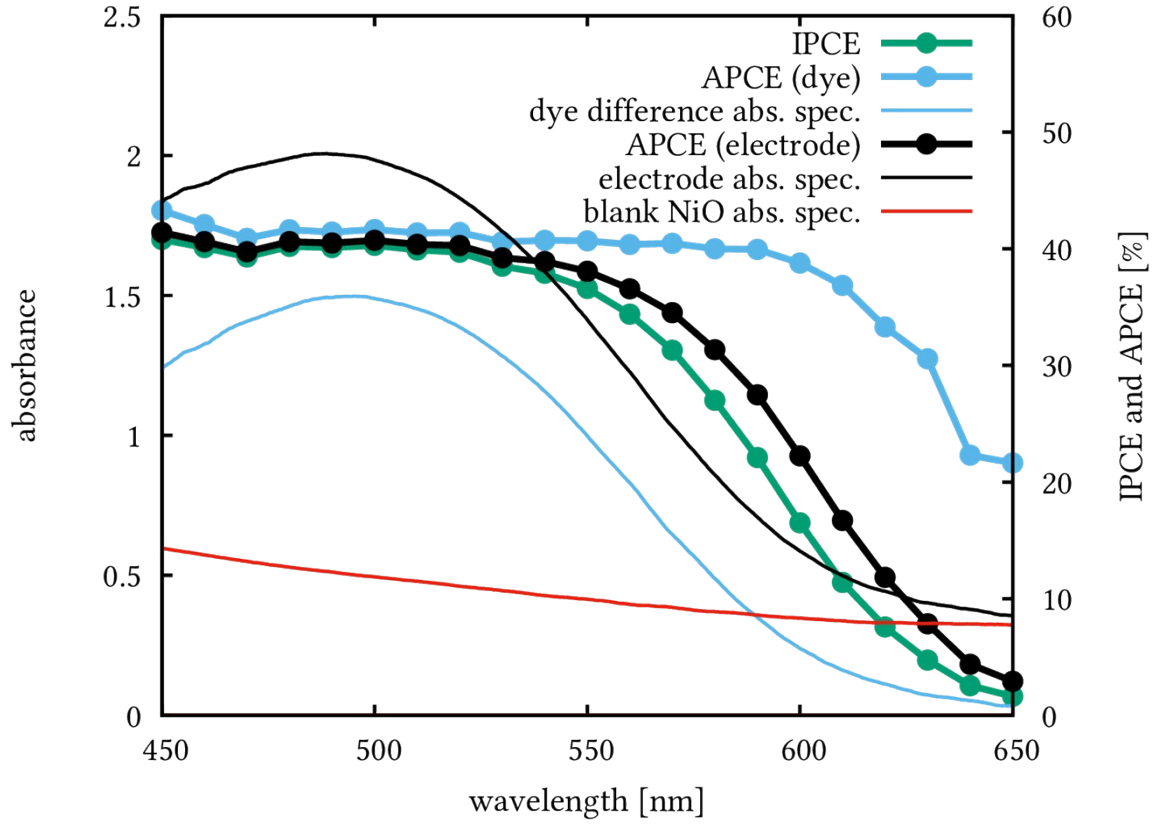

Figure S2. [**5d**] Example measurement: The blank NiO film exhibits a broad unstructured absorption spectrum (red). Upon sensitization the prominent charge-transfer band of the dye on the NiO film with its maximum close to 500 nm is revealed in the absorption spectrum (black). Subtraction of the blank NiO spectrum from the electrode spectrum yields the difference spectrum representing the dye on the NiO (blue). APCE spectra related to the electrode absorption (black lines–points) and related to the dye on the surface (blue lines–points) were derived from the IPCE spectrum (green).

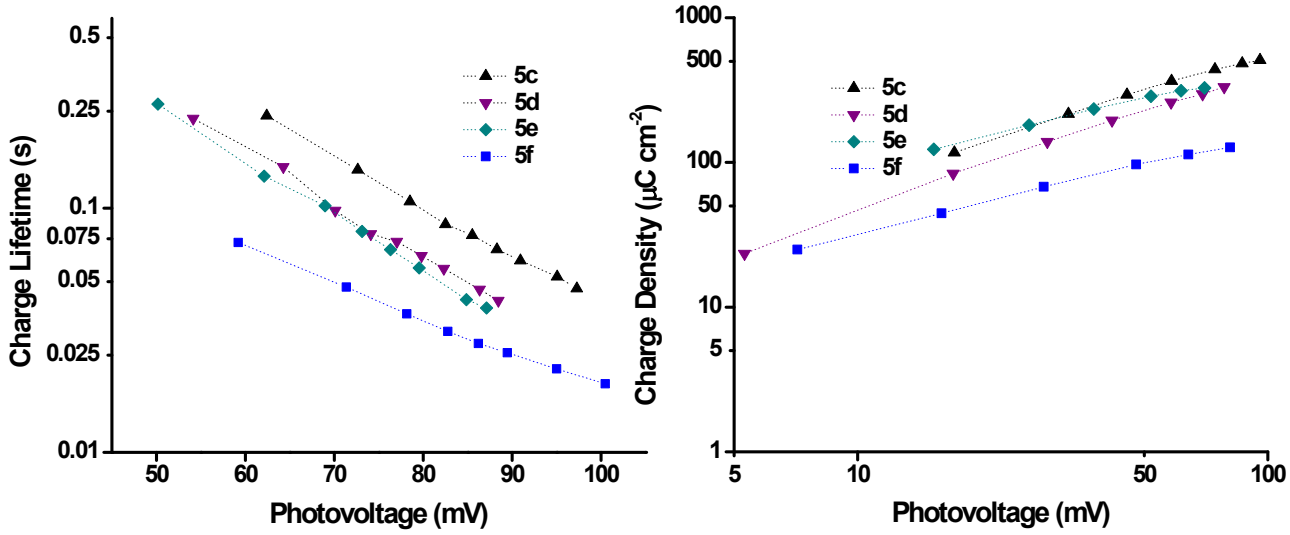

Figure S3. Plots of charge lifetime *vs.* photovoltage (left) and of extracted charge density *vs.* photovoltage (right) for samples prepared from commercial NiO pastes.

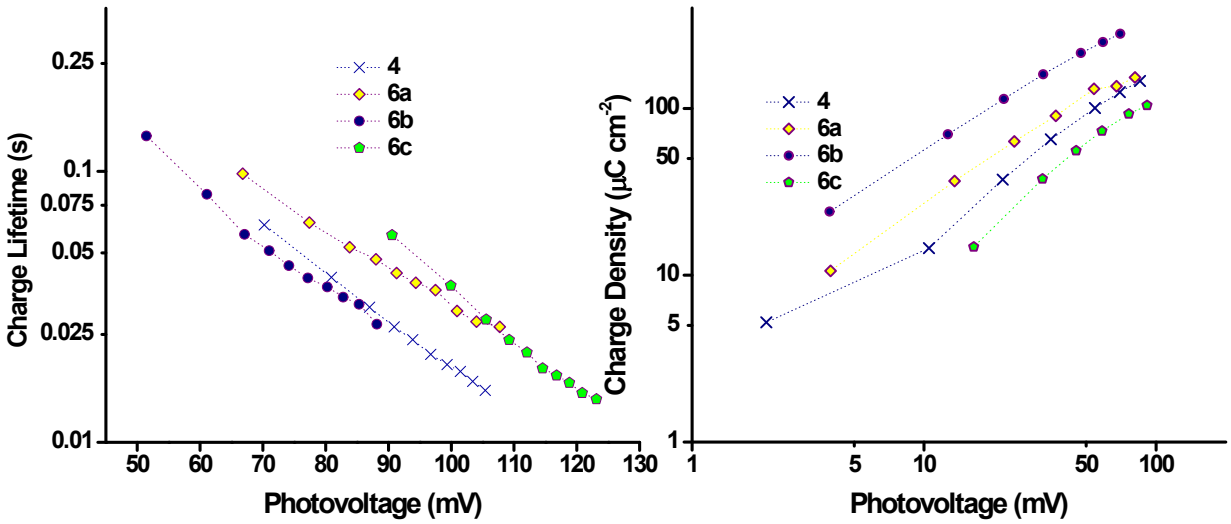

Figure S4. Plots of charge lifetime *vs.* photovoltage (left) and of extracted charge density *vs.* photovoltage (right) for Li doped samples.

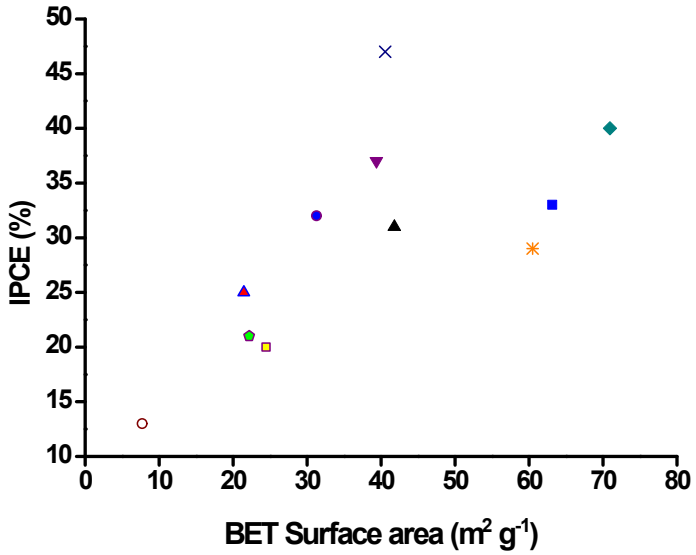

Figure S5. A plot of IPCE *vs.* BET specific surface area.

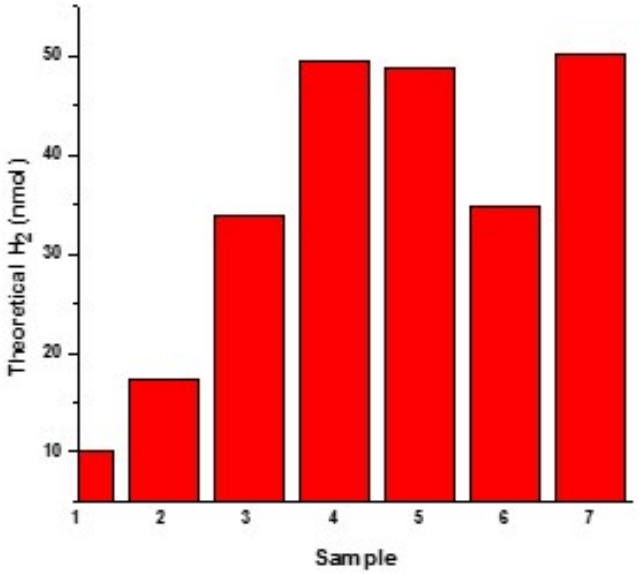

Figure S6. A plot of theoretical H_2 calculated from the total charge under irradiation in Figure 10.