

Supporting Information

Ligand-free preparation of polymer/CuInS₂ nanocrystal films and the influence of 1,3-benzenedithiol on their photovoltaic performance and charge recombination properties

Thomas Rath,^{1,*} Dorothea Scheunemann,² Roberto Canteri,³ Heinz Amenitsch,⁴ Jasmin Handl,¹ Karin Wewerka,⁵ Gerald Kothleitner,⁵ Simon Leimgruber,¹ Astrid-Caroline Knall,¹ and Saif A. Haque⁶

¹ Institute for Chemistry and Technology of Materials (ICTM), NAWI Graz, Graz University of Technology, Stremayrgasse 9, 8010 Graz, Austria

² Energy and Semiconductor Research Laboratory, Department of Physics, Carl von Ossietzky University of Oldenburg, Carl-von-Ossietzky-Strasse 9–11, 26129 Oldenburg, Germany

³ Fondazione Bruno Kessler - Center for Materials and Microsystems, Via Sommarive 18, I-38123 Povo (Trento), Italy

⁴ Institute for Inorganic Chemistry, NAWI Graz, Graz University of Technology, Stremayrgasse 9, 8010 Graz, Austria

⁵ Institute for Electron Microscopy and Nanoanalysis and Center for Electron Microscopy, Graz University of Technology, NAWI Graz, Steyrergasse 17, 8010 Graz, Austria

⁶ Department of Chemistry and Centre for Plastic Electronics, Imperial College London, Imperial College Road, London, SW7 2AZ, UK

* Corresponding author address: Institute for Chemistry and Technology of Materials (ICTM), NAWI Graz, Graz University of Technology, Stremayrgasse 9, 8010 Graz, Austria;
Email: thomas.rath@tugraz.at

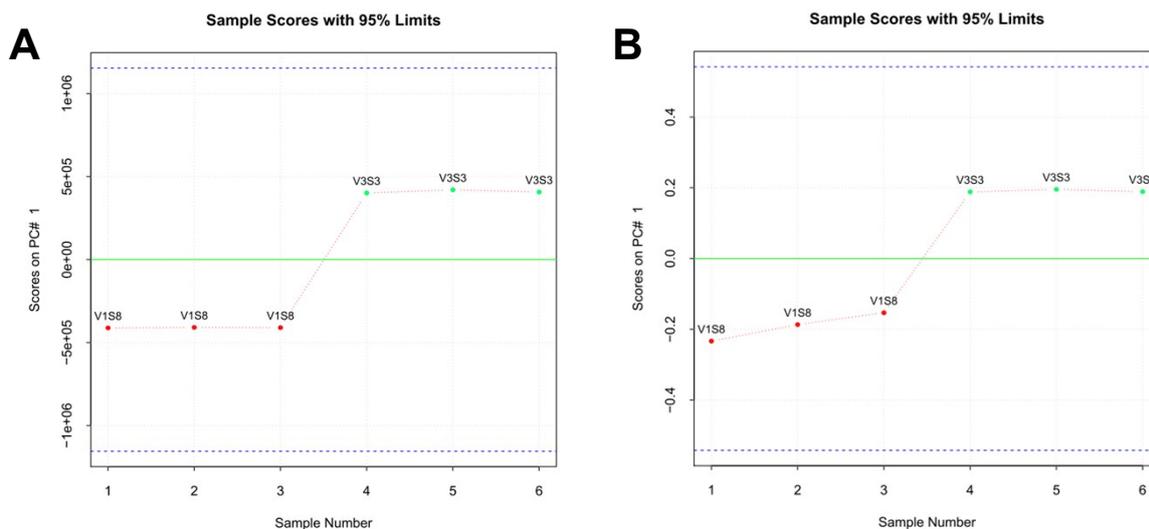


Fig. S1 Scores plots (A: negative ions, B: positive ions) extracted from the ToF-SIMS measurements. The red dots represent the non-modified sample, the green dots the sample modified with 1,3-benzenedithiol.

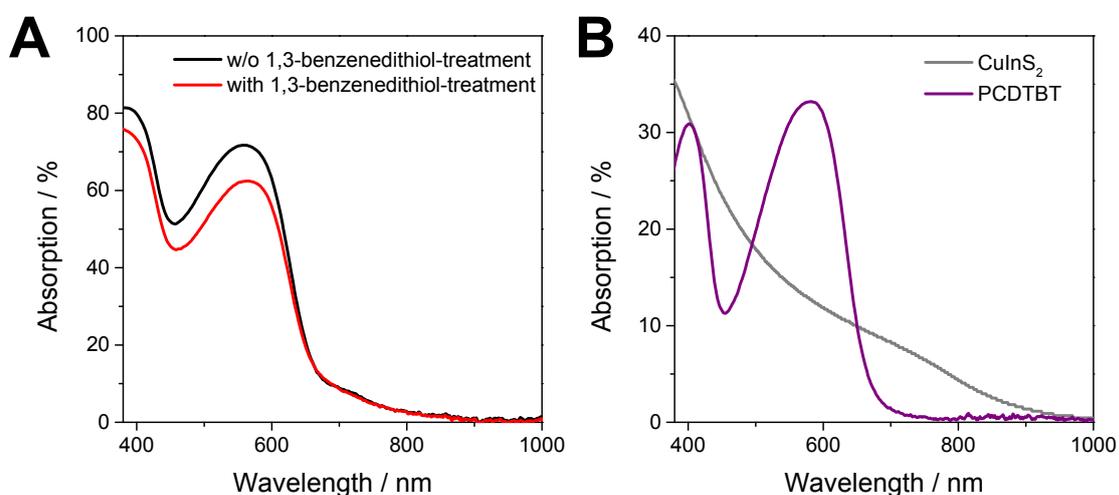


Fig. S2 (A) UV-Vis absorption spectra of the mp-TiO₂/CIS/PCDTBT films on glass (with and without 1,3-benzenedithiol treatment) used for the transient absorption spectroscopy measurements; (B) UV-Vis spectra of pristine PCDTBT and CuInS₂ thin films on glass.

For the determination of the absorption spectra, transmission and reflection spectra were recorded on a Shimadzu 2600 spectrophotometer equipped with an ISR-2600Plus integrating sphere attachment.

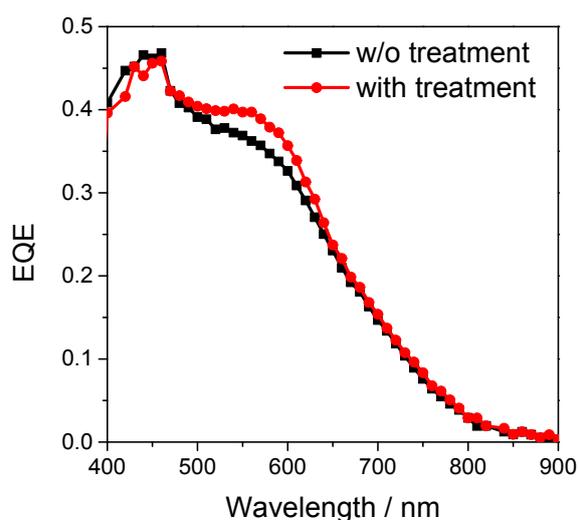


Fig. S3 EQE spectra of PCDTBT/CuInS₂ solar cells without and with 1,3-benzenedithiol modification.

The EQE spectra were acquired using a MuLTImode 4 monochromator (Amko) equipped with a 75 W xenon lamp (LPS 210-U, Amko), a lock-in amplifier (Stanford Research Systems, Model SR830), and a Keithley 2400 source meter. The monochromatic light was chopped at a frequency of 30 Hz and the measurement setup was spectrally calibrated with a silicon photodiode (Newport Corporation, 818-UV/DB).

Table S1 Characteristic solar cell parameters of PPD–BDT/CuInS₂ solar cells with and without 1,3-benzenedithiol modification (average values and standard deviations are calculated from the five best devices each)

	V_{oc} / V	$J_{sc} / \text{mA}/\text{cm}^2$	FF	PCE / %
w/o modification	0.498 ± 0.018	8.22 ± 1.02	0.44 ± 0.05	1.81 ± 0.36
with modification	0.494 ± 0.010	10.06 ± 0.23	0.51 ± 0.02	2.54 ± 0.13

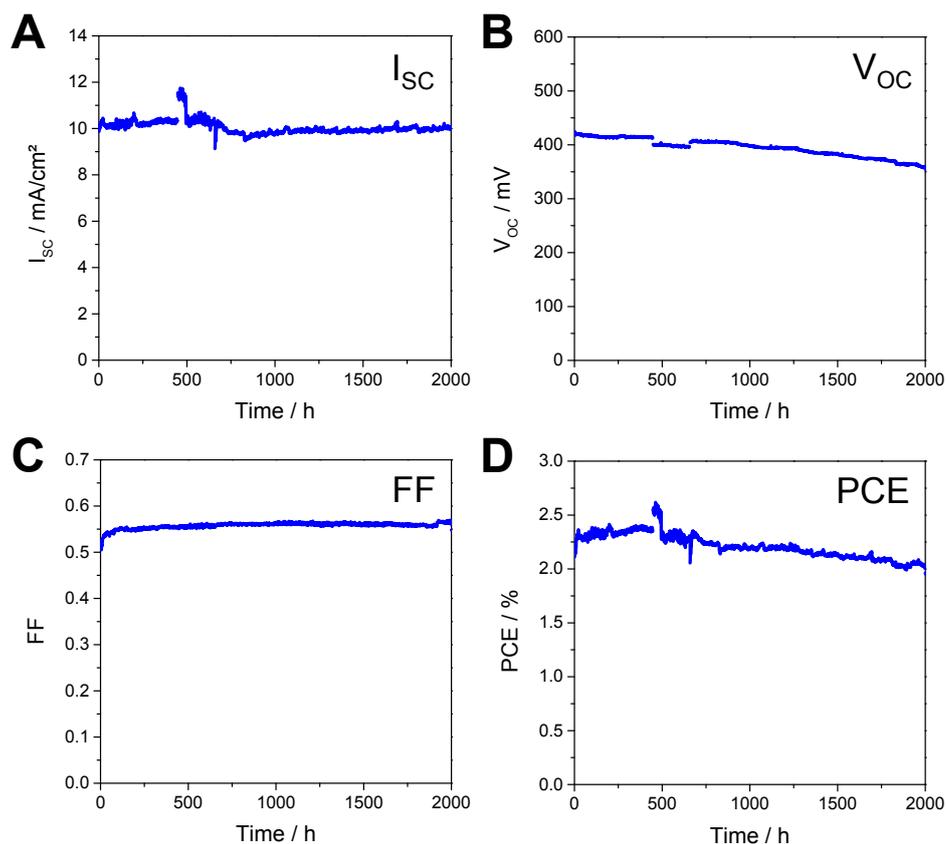


Fig. S4 Results of a 2000 h stability test of a PPD-BDT/CuInS₂ solar cell modified with 1,3-benzenedithiol. The slight artefacts present in the characteristic solar cell data around 500 h are due to irregularities of the measuring setup during this time period.

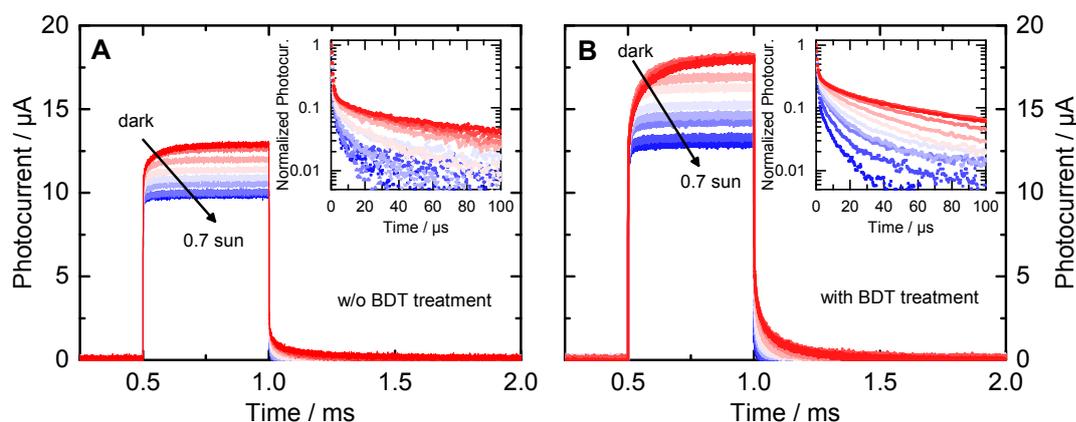


Fig. S5 TPC signals as a function of white-light background illumination intensity (dark to 0.7 suns, zero bias voltage) for PCDTBT/CuInS₂ solar cells (A) without and (B) with 1,3-benzenedithiol modification. The insets show the corresponding normalized photocurrent transients.