

Supplementary Information

Improved sensitization of zinc oxide nanorods by cadmium telluride quantum dots through charge induced hydrophilic surface generation

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Section I: Cdte QD size measurement

The synthesized cadmium telluride (CdTe) quantum dots were characterized by dynamic light scattering technique using CILAS Nano DS dual scattering particle size analyzer. The resulting size distribution is as shown below:

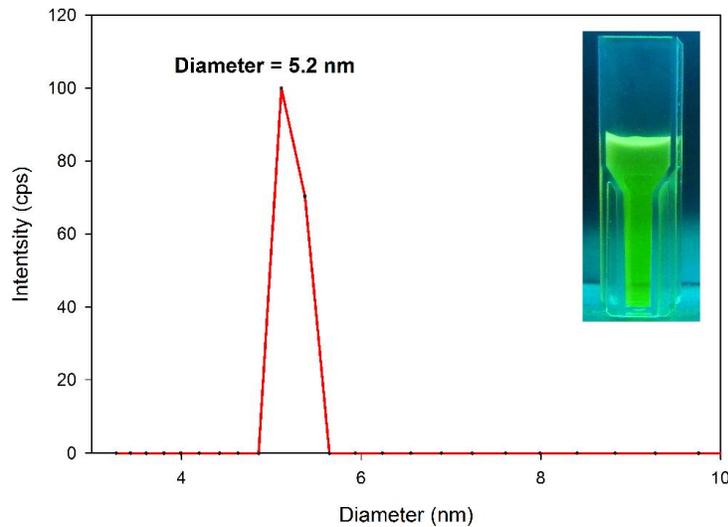


Figure S1: CdTe quantum dot (500nm absorption) size distribution analyzed by dual light scattering technique, showing quantum dot diameter ranging from 5.2 nm to 5.8 nm. Inset shows the fluorescence of the quantum dots under UV light illumination

Section II: Infrared spectroscopy

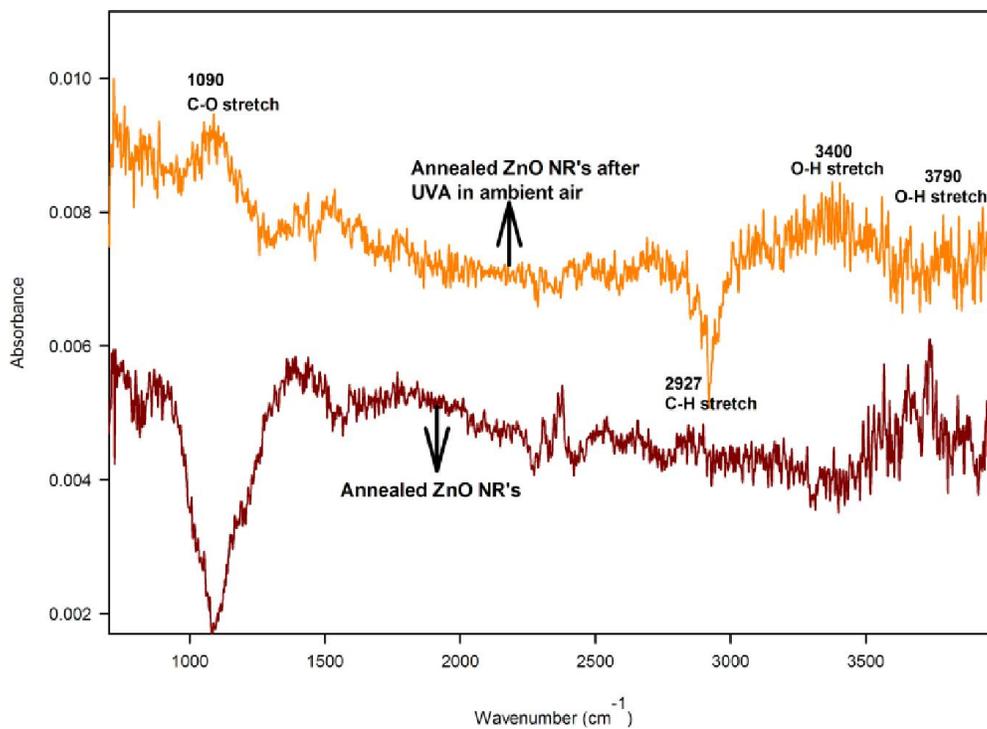


Figure S2: Infrared absorption spectra of air annealed ZnO NR's before and after UV annealing in ambient air. The spectra shows the increase in surface OH concentration, organic impurity degradation and attachment of CO₂ on the NR surfaces after UV annealing in air

UV annealing induced defects have been known to bind with atmospheric moisture and other compounds [1, 2], which was studied by vibrational spectroscopy. Vibrational spectra of air annealed ZnO after UV exposure showed distinct changes in absorption peaks at 1090 cm⁻¹ attributed to C-O stretch of carbon dioxide (CO₂) adsorbed on ZnO [3], 2927 cm⁻¹ attributed to C-H stretch of organic impurities adsorbed from the ambient [4] and a wide absorption peak between 3200 – 3600 cm⁻¹ attributed to adsorbed surface hydroxyls [5] as shown in **Figure S2**. Absorption peak at 1090 cm⁻¹ could be prevalent due to the adsorption of CO₂ at oxygen vacancy sites after UV exposure [1]. The oxygen atom of CO₂ binds to the vacancy sites, orienting the molecule in a tridentate bonding, where both oxygen atoms reorient close to vacancy positions, while the carbon atom binds to a surface oxygen with all three C-O bond lengths nearly equal [3]. The longer C-O bond lengths dominate the asymmetric stretch frequency of the adsorbate and could be the source of the 1090 cm⁻¹ stretch. This is again indicative of the formation of oxygen vacancies upon UV annealing, while it also suggests that not all defect sites are populated by hydroxyl groups. The reduction in the C-H stretch at 2927 cm⁻¹ suggests the degradation of organic contaminants on the surface upon UV annealing.

Section III: Solar cell IV curves

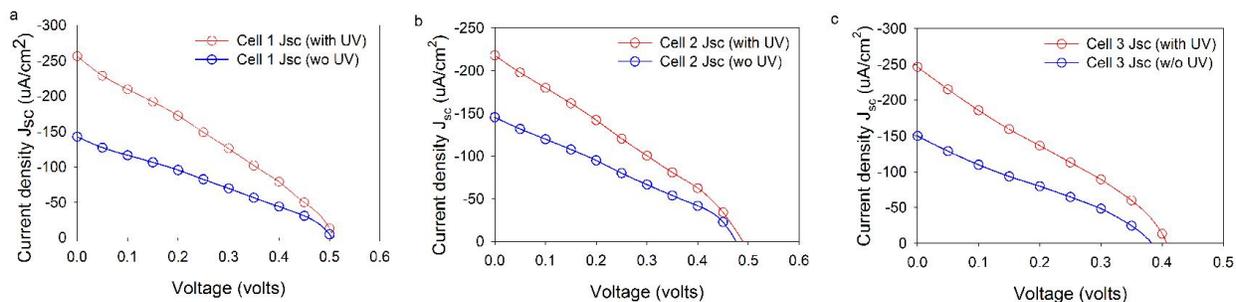


Figure S3: (a, b and c) I-V characteristics of 3 different QDSSC’s, where each was made with and without UV exposure of the photo-electrode. The blue lines show the I-V curve without UV exposure, while the red lines show the increase in the current and voltage after UV exposure. In all cases there was a substantial increase in the short circuit current of the cell, while enhancements in the open circuit voltage varied to a small degree.

Section IV: I-V characteristics for multiple QD deposition on NO nanorod supports showing improved current density

Table S1: IV characteristics of CdTe QD solar cells made from UV annealed ZnO NR based PE’s showing a increase in both V_{oc} and J_{sc} for multiple QD deposition cycles

Photo-electrode	Open Circuit voltage (volts)	Current Density (mA/cm ²)
DEZ NR’s	0.52V	3.75 mA/cm ²

References

- [1] U. Burghaus, Surface science perspective of carbon dioxide chemistry—Adsorption kinetics and dynamics of CO₂ on selected model surfaces, *Catal. Today* 148 (2009) 212-220.
- [2] R.-D. Sun, A. Nakajima, A. Fujishima, T. Watanabe, K. Hashimoto, Photoinduced Surface Wettability Conversion of ZnO and TiO₂ Thin Films, *J. Phys. Chem. B* 105 (2001) 1984-1990.
- [3] J. Kossmann, G. Rossmuller, C. Hattig, Prediction of vibrational frequencies of possible intermediates and side products of the methanol synthesis on ZnO(000 $\bar{1}$) by ab initio calculations, *J. Chem. Phys.* 136 (2012) 034706.
- [4] T. Nakajima, H. Miyata, Y. Kubokawa, Infrared studies of intermediates in the oxidation of propene on ZnO using ¹⁸O₂, *J. Chem. Soc., Farad. Trans.* 81 (1985) 2409-2419.
- [5] T. Noguchi, FTIR detection of water reactions in the oxygen-evolving centre of photosystem II, *Philos. T R Soc. B* 363 (2008) 1189-1195.