

Supporting Information for:

A Comparison of the Behavior of Single Crystalline and Nanowire Array ZnO Photoanodes

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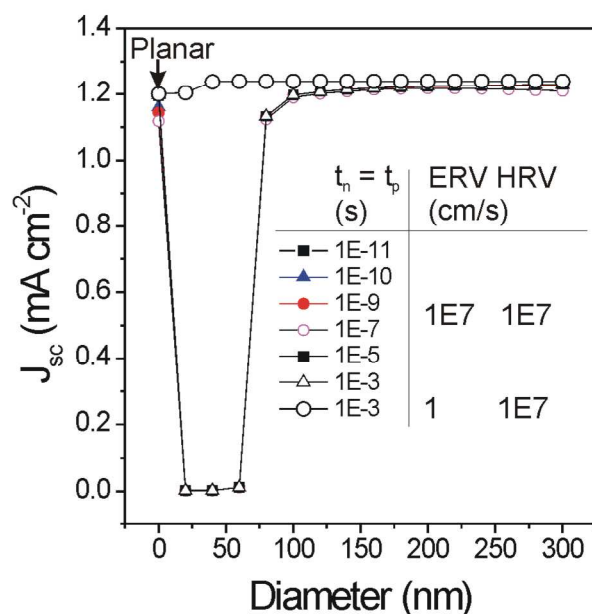


Figure S1. Simulated short circuit current densities under 1-sun illumination for ZnO nanowires with varying diameter, electron and hole lifetime, and interfacial electron and hole recombination velocities. Despite long carrier lifetimes of 1 ms large J_{sc} values are not observed in wires with $d < 75$ nm. However, when the electron recombination velocity is reduced, simulating a ‘hole-selective’ contact characteristic of dye-sensitized solar cells, large J_{sc} values are obtained even at small wire diameters where very little electric field is present (See **Figure S2**).

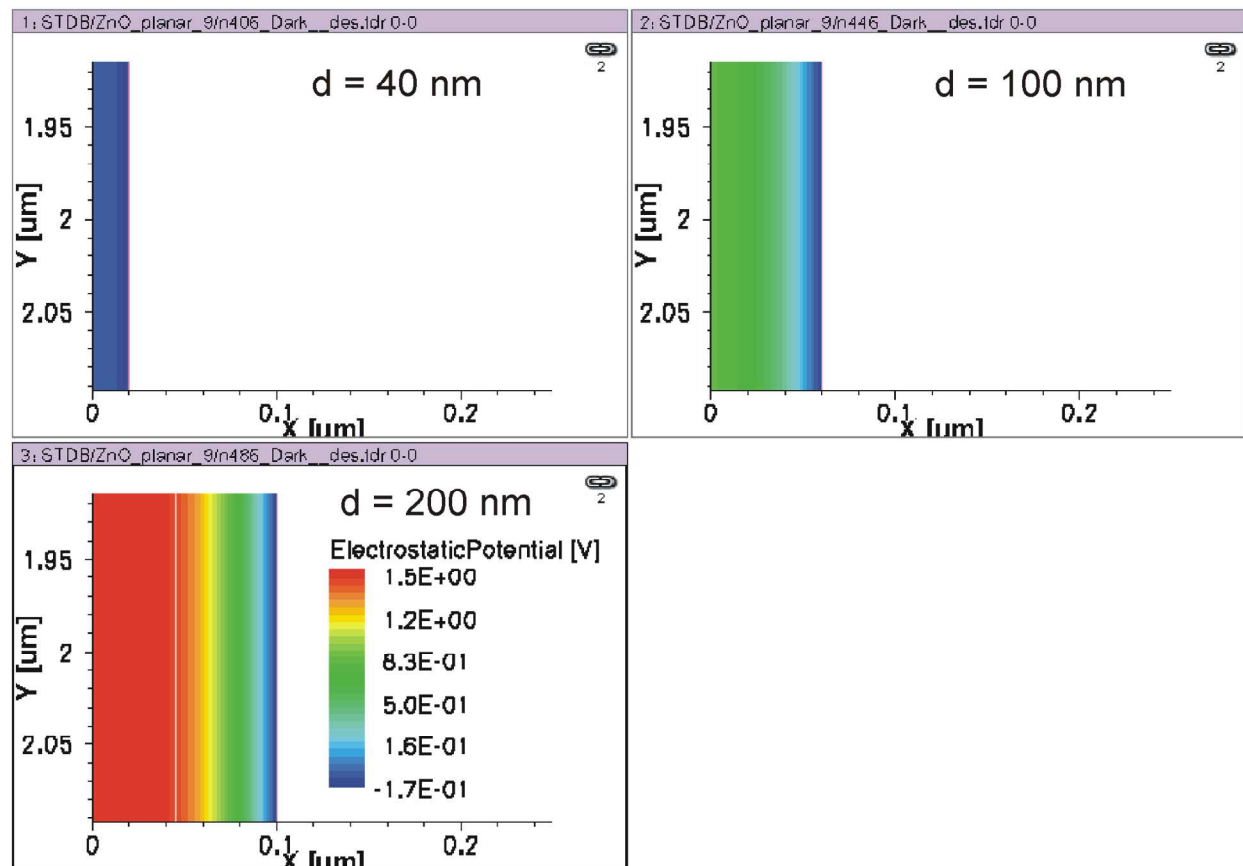


Figure S2. Simulated electrostatic potential in the dark, plotted vs. spatial coordinates of cross-sections of one half of ZnO nanowires with diameters of 40 nm, 100 nm, and 200 nm.

Table S1. Parameters for the device physics simulation

Parameter	Value
Band Gap	3.3 (eV)
Electron Affinity	3.7 (eV)
Electron DOS	$4.0E18$ (cm^{-3})
Hole DOS	$1.8E19$ (cm^{-3})
Electron Mobility	50 ($\text{cm}^2 \text{V}^{-1} \text{s}^{-1}$)
Hole Mobility	10 ($\text{cm}^2 \text{V}^{-1} \text{s}^{-1}$)
Electron lifetime	$1E-9$ (s)
Hole lifetime	$1E-9$ (s)
Electron Recombination Velocity	$1E7$ (cm s^{-1})
Hole Recombination Velocity	$1E7$ (cm s^{-1})

Index of refraction data and absorption coefficient data were taken from Ref 1.

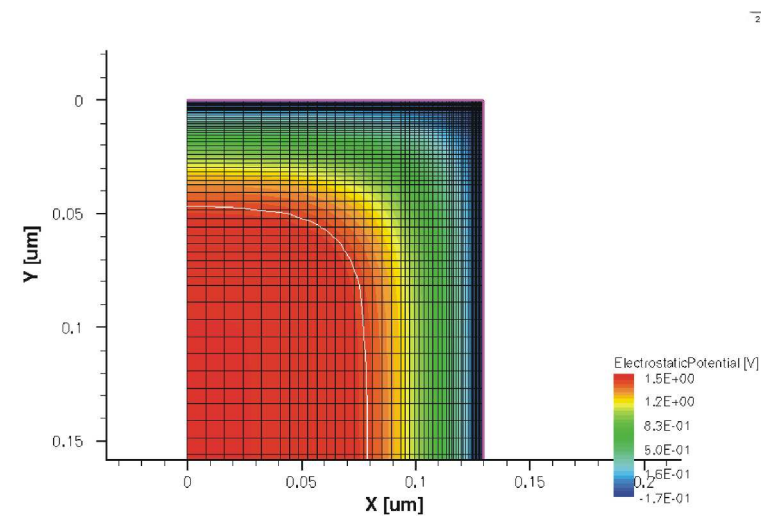


Figure S4. Example of the simulation mesh used in device physics simulations.

References:

- (1) Yoshikawa, H.; Adachi, S. *Japanese Journal of Applied Physics* **1997**, 36, 6237.

Complete Reference 2:

2. Boettcher, S. W.; Warren, E. L.; Putnam, M. C.; Santori, E. A.; Turner-Evans, D.; Kelzenberg, M. D.; Walter, M. G.; McKone, J. R.; Brunschwig, B. S.; Atwater, H. A.; Lewis, N.S., *J. Am. Chem. Soc.* **2011**, 133, 1216-1219.