

Supporting information

Antireflective Coatings of ZnO Quantum Dots and their Photocatalytic Activity

T. Jesper Jacobsson* and Tomas Edvinsson

Dept. of Chemistry - Ångström Laboratory, Uppsala Univ., Box 538, 75121 Uppsala, Sweden

Jesper.jacobsson@kemi.uu.se, +46 (0)70-5745116

1. Summary of key data for the photodecomposition of methylene blue

Table S.1. Summary of key data concerning the photodecomposition of methylene blue

Sample	E _g [eV]	d [Å]	Min _{abs} [a.u]	Max _{abs} [a.u]	nph s ⁻¹ abs	A ₂₄₀ /A ₀
1	3.60	37	-0.20	1.14	2.1·10 ¹⁵	0.0244
2	3.56	40	-0.24	0.86	2.5·10 ¹⁵	0.1591
3	3.51	44	-0.20	0.61	3.0·10 ¹⁵	0.4254
4	3.48	47	-0.25	0.58	3.2·10 ¹⁵	0.5204
5	3.46	51	-0.24	0.73	3.5·10 ¹⁵	0.4446
6	3.44	55	-0.22	0.54	3.7·10 ¹⁵	0.5681
7	3.41	61	-0.20	1.04	4.0·10 ¹⁵	0.3273
8	3.40	62	-0.16	1.27	4.1·10 ¹⁵	0.3002
9	3.39	65	-0.17	0.66	4.2·10 ¹⁵	0.3428
Substrate	-	-	-	-	-	-
Blank	-	-	-	-	-	-

2. Photodecomposition of methylene blue, additional figures

What follows below is the full set of figures corresponding to figure 6 in the main article

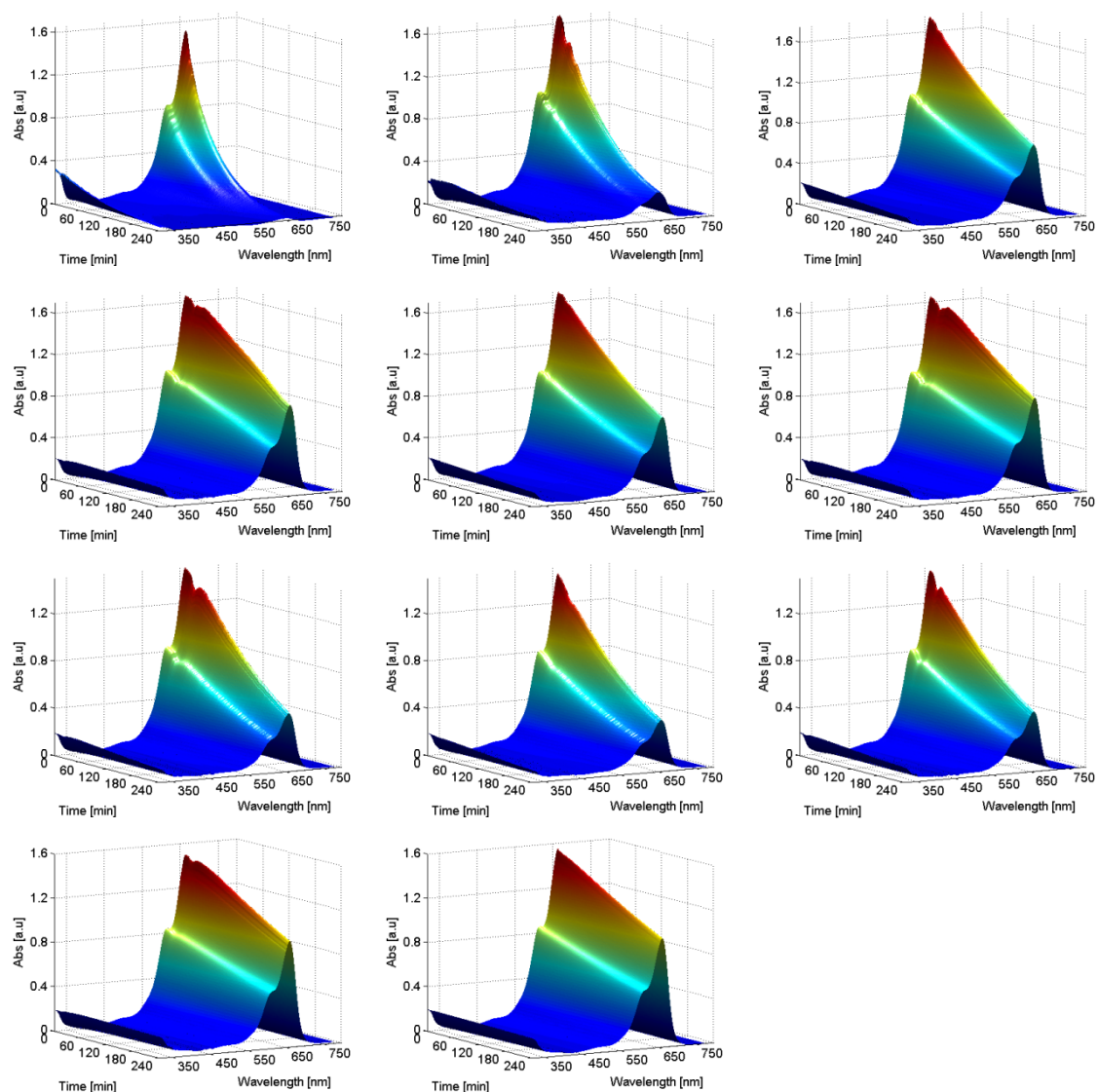


Figure S.1. By starting at the upper left corner, going from left to right and ending at the lower right corner is figures for sample 1 to 9, the substrate and the blank sample. 3D surfaces corresponding to absorption against wavelength and reaction time during illumination of a 4.5 ml cuvette with 10 μM methylene blue and a FTO substrate with a thin film of ZnO quantum dots.

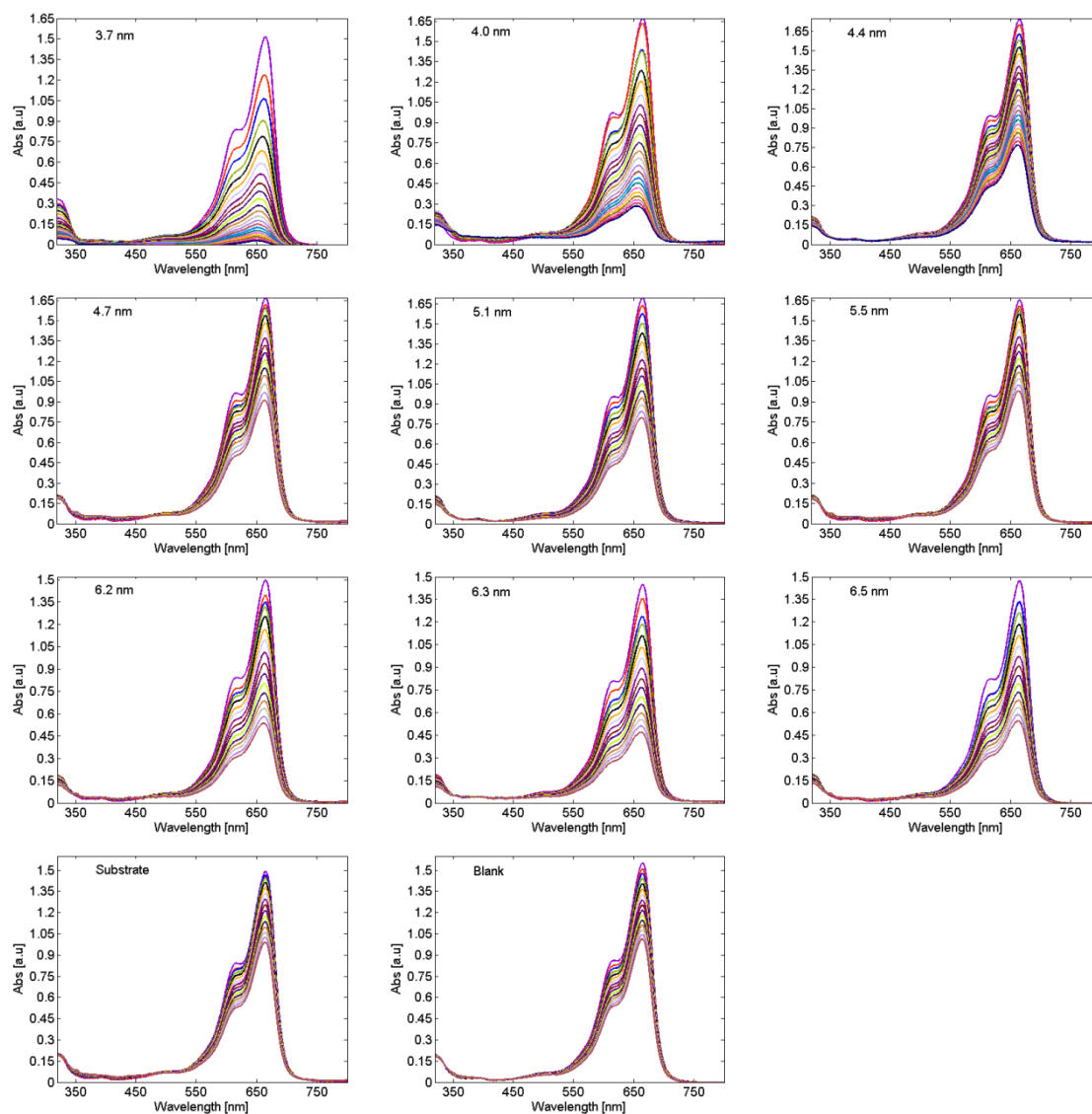


Figure S.2 Absorption against wavelength for different reaction times. These are two dimensional projections of the individual figures in figure S.1.

Table S.2. The R^2 values for a linear fit to data in figure S.3

Sample	1	2	3	4	5	6	7	8	9	Substrate	Blank
d [Å]	37	40	44	47	51	55	62	63	65	-	-
R^2	0.839	0.957	0.9914	0.9895	0.9952	0.9862	0.993	0.9866	0.9921	0.9993	0.9906

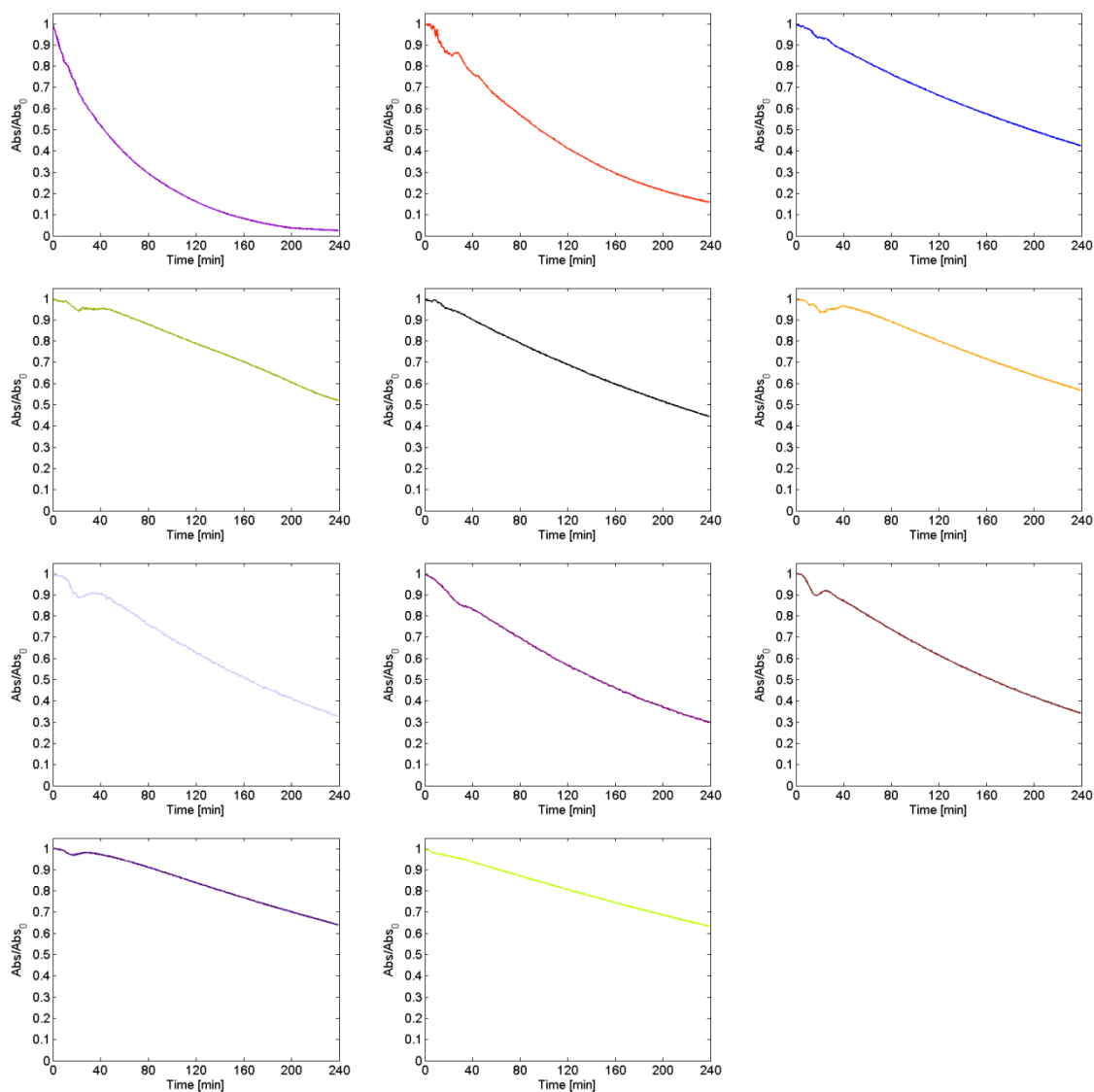


Figure S.3. Maximum absorption normalized with the absorption at the start of the experiment against reaction time. This corresponds to the ridges in figure S.1 and the maximums in figure S.2. According to Lambert-Beers law this corresponds to the fraction of methylene blue remaining in the solution as a function of time during illumination.

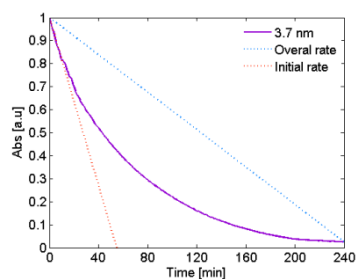


Figure S.4. A version of figure S.3.a but with initial and overall reaction rate marked.

3. Normalization of the sun lamp

In order to simulate the solar AM 1.5 spectrum we were using a xenon lamp with an air mass filter. This gives a spectrum that for most purpose is reasonable close to the solar spectrum, but in order to get an accurate measure of the quantum efficiency, the photon flux of the lamp in the laboratory needs to be known. This have been determined as illustrated by figure S.5

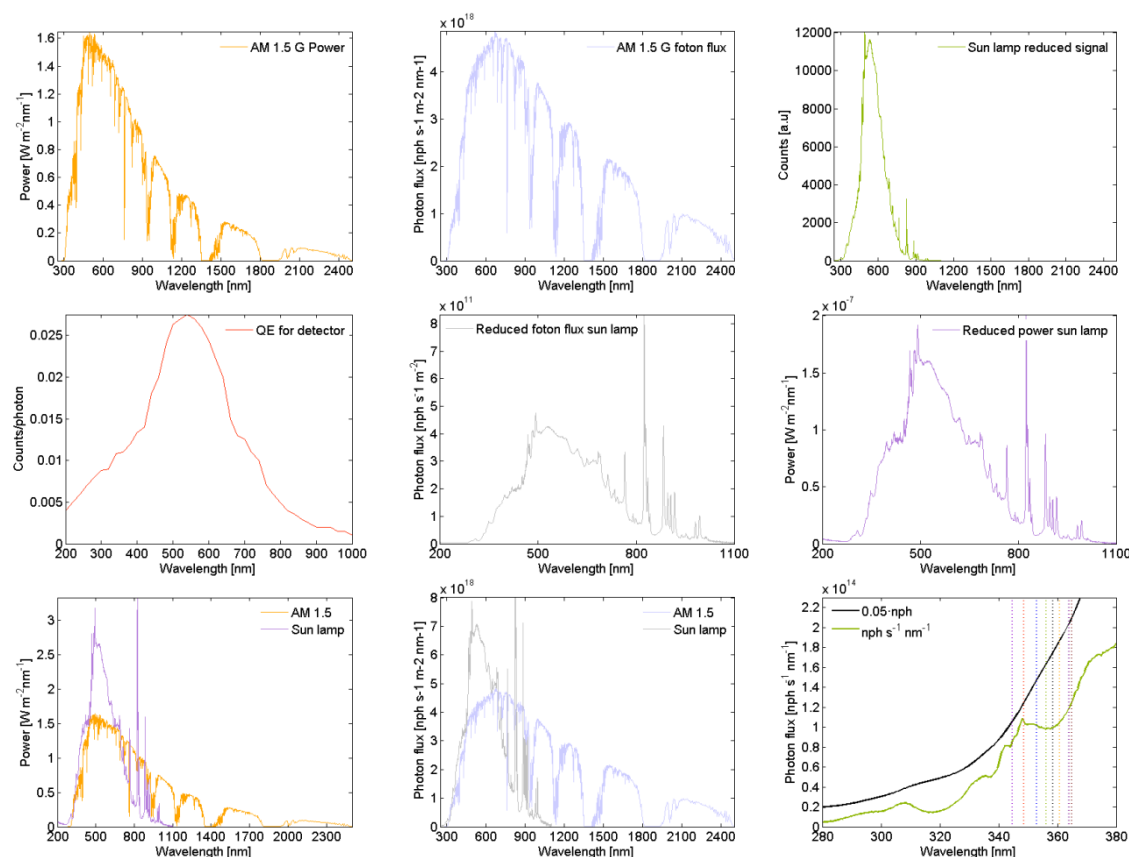


Figure S.5.

(a) Incident power from the sun. AM 1.5 G. Downloaded from NREL.

(b) The corresponding photon flux for the AM 1.5 G spectrum.

(c) The spectrum for the sun lamp measured by our UV-vis detector. The detector is not made for measuring one sun intensity, wherefore the measurement have been done at an angle from the lamp in order to reduce the intensity and prevent the detector from saturation.

(d) The quantum efficiency of the detector as specified by the manufacturer.

(e) The photon flux from the sun lamp as measured in (c) but corrected for the QE in the detector.

(f) The incident power corresponding to (e).

(g) Normalized spectra from the sun lamp with respect to AM 1.5. Our detector only detects up to 1100 nm and we have assumed that the intensity in the IR are approximately the same for the sun lamp and the AM 1.5 spectrum.

(h) The corresponding normalized photon flux from the sun lamp compared to the AM 1.5 spectrum.

(i) Integrated photon flux from the sun lamp up to wavelengths corresponding to the band gaps.

4. Summary of key data for solar water splitting experiments

Table S.3. Summary of key data concerning the solar water splitting experiments

Sample	E_g [eV]	d [Å]	Min_{abs} [a.u.]	Max_{abs} [a.u.]	I_{max} at ca 0.5 V vs NHE [mA/cm ²]	Absorbed n_{ph} [s ⁻¹]
1	3.65	34	-0.26	0.12	0.019	$2.1 \cdot 10^{15}$
2	3.59	37	-0.27	0.58	0.024	$2.5 \cdot 10^{15}$
3	3.51	44	-0.19	0.70	0.046	$2.9 \cdot 10^{15}$
4	3.48	47	-0.19	0.67	0.063	$3.2 \cdot 10^{15}$
5	3.45	52	-0.20	1.39	0.064	$3.5 \cdot 10^{15}$
6	3.43	55	-0.21	1.29	0.062	$3.7 \cdot 10^{15}$
7	3.40	63	-0.20	1.04	0.034	$4.0 \cdot 10^{15}$

5. Absorption data for water splitting experiments

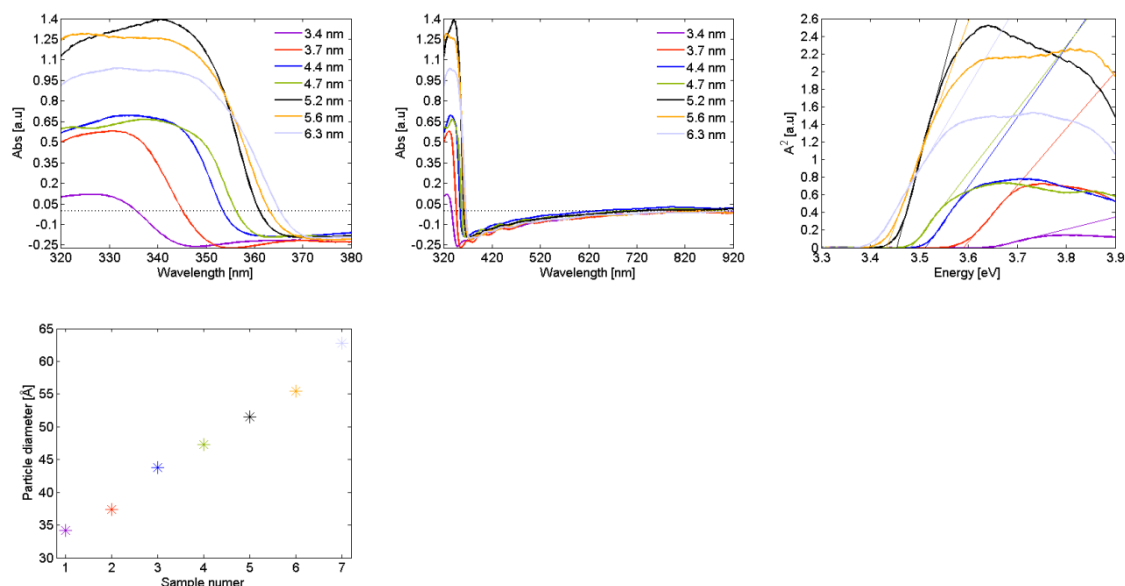


Figure S.6 (a) Absorption as a function of wavelength of the samples which were used for photodegradation of methylene blue. (b) Absorption in a larger wavelength interval demonstrating the antireflective behavior in the visible region (c) Determination of the corresponding band gaps by plotting the square of the absorption against photon energy. (d) Particle diameter determined from E_g and equation 1.

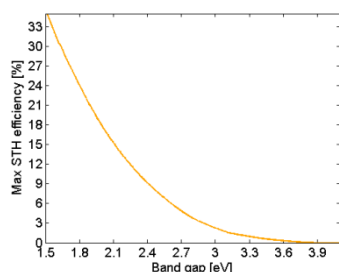


Figure S.7. Theoretical maximum solar to hydrogen efficiency as a function of band gap. Based on the solar AM 1.5 G spectrum

6. Water splitting experiments

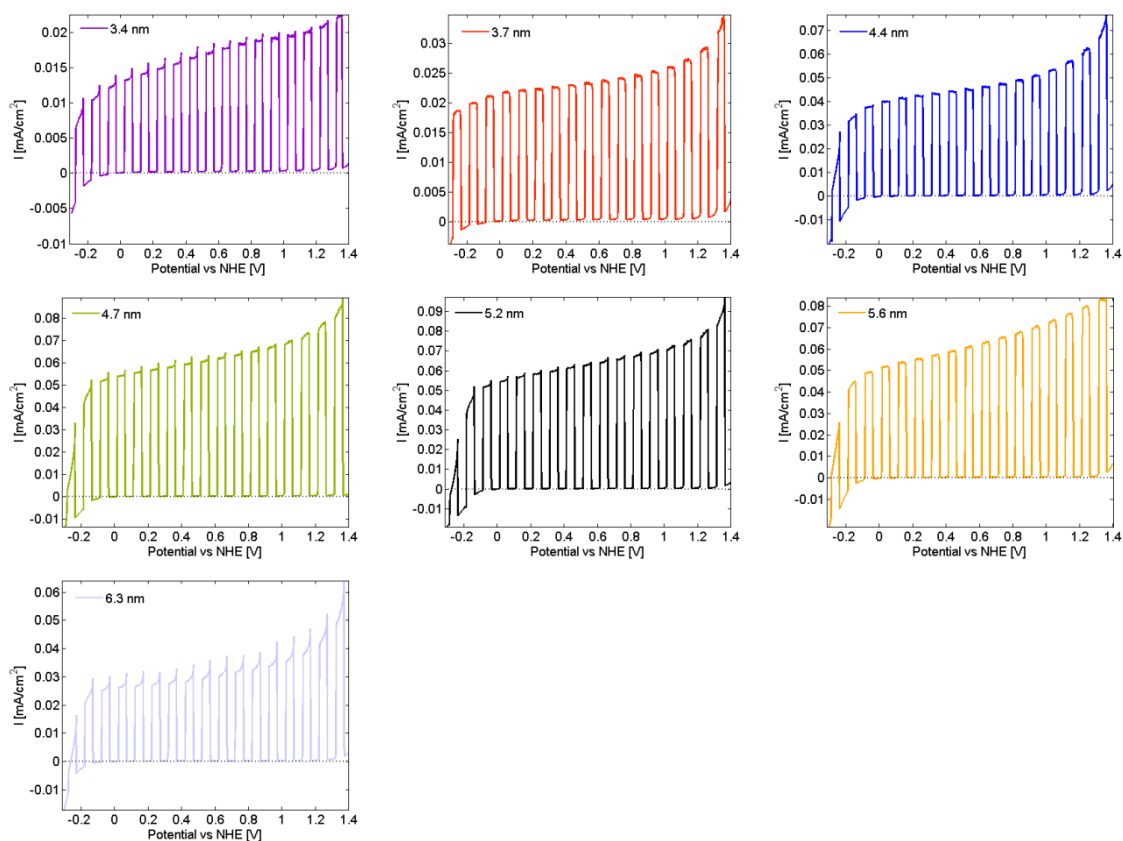


Figure S.8. Current density as a function of potential under chopped simulated AM 1.5 illumination for the entire set of samples. Illumination from the front side.

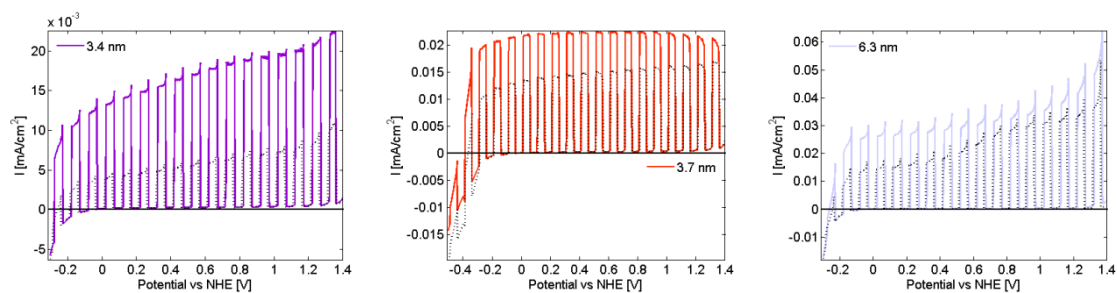


Figure S.9. Current density as a function of potential under chopped simulated AM 1.5 illumination from both the front and back side for some of the samples. The black lines are for back side illumination.