Supplementary Material (ESI) for
Catalysis Science & Technology
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Supporting Information

Completely Integrated Wirelessly-Powered Photocatalyst Spheres as a Novel Means to Perform Heterogeneous Photocatalytic Reactions

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1. Results and Discussion

1.1. Characterization of the coated WLE

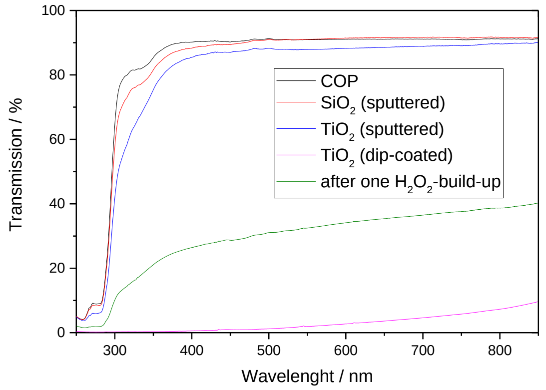

Figure S1. Transmission spectra of the individual layers / coating steps.

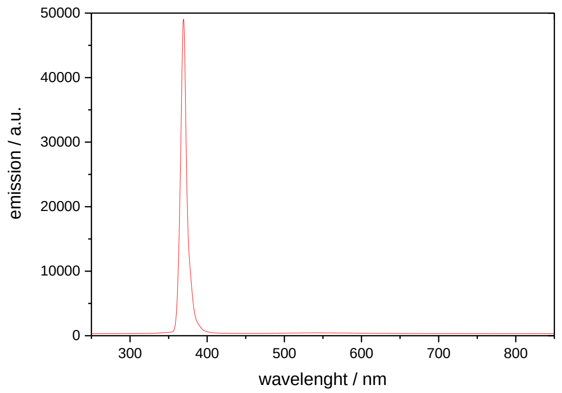

Figure S2. Emission spectrum of a SiO_2-coated WLE.

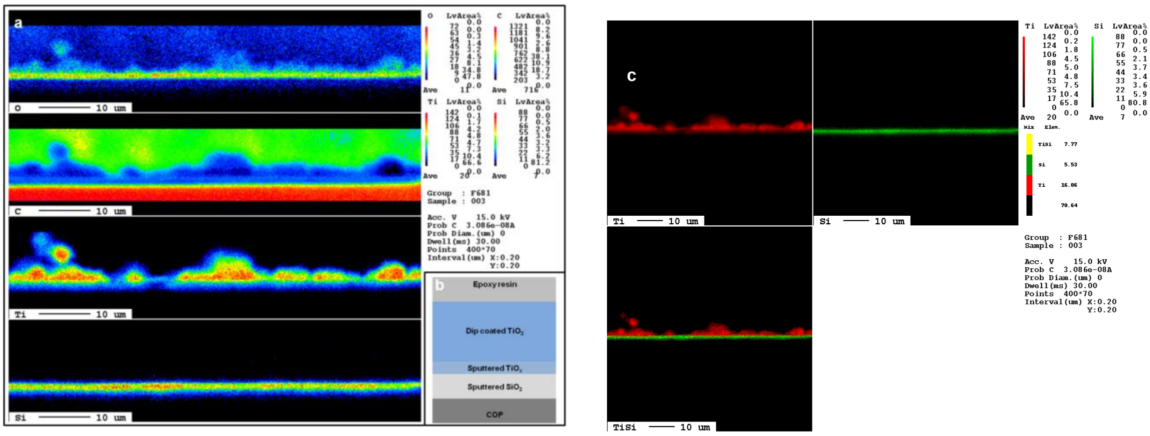

Figure S3. EPMA/WDS element mapping of a cross section cut of a coated COP sheet (a), schematic view of the mapped layers (b) and mapping pictures with different colours for Ti and Si with an overlay to see the separation of the layers (c).

1.2. Photocatalytic H_2O_2 production with WLE

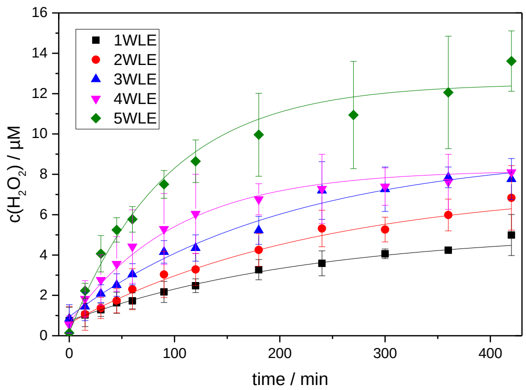

Figure S4. Concentration-time-profiles for the photocatalytic H_2O_2 generation with different numbers of WLE. Reaction conditions were as follows: 1-5 coated WLE, 30 ml 0.1M phosphate buffer, pH = 3, 60 mL min^{-1} O_2 bubbling. Solid lines represent a fit using the kinetics described by Kormann *et al.*[1].

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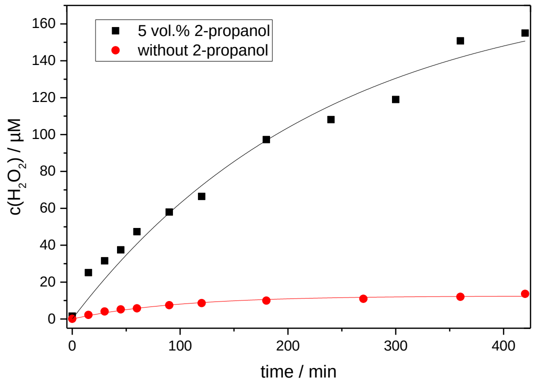
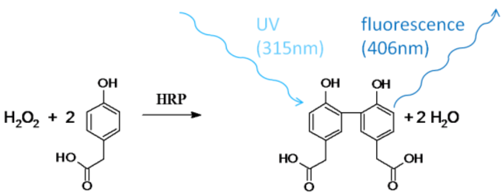


Figure S5. Comparison of the concentration-time-profiles of the photocatalytic H_2O_2 generation with (black) and without (red) the use of 2-propanol (5. vol. %) as sacrificial electron donor. Reaction conditions were as follows: 5 coated WLE, 30 ml 0.1M phosphate buffer, pH = 3, 60 mL min^{-1} O_2 bubbling. Solid lines represent a fit using the kinetics described by Kormann *et al.*[1].

Table S1. Kinetic data for H_2O_2 generation reactions.

n WLE	Photon flux density µE L^{-1} min^{-1}	k_B µM min^{-1}	ξ^1 %	k_B (iPrOH) µM min^{-1}	ξ^1 %	k_B (suspension) µM min^{-1}	ξ^1 %
1	47.8182	0.0226	0.0946			0.0896	0.3748
2	113.9917	0.0314	0.0550				
3	135.2603	0.0440	0.0650				
4	189.0114	0.0817	0.0864				
5	237.2703	0.1349	0.1138	0.7695	0.6486	0.2042	0.1720

[1]assuming two photons are required for each conversation.



Scheme S1. Reaction scheme of HRP catalyzed dimerisation of *p*-hydroxyphenylaceticacid as probe reaction for H_2O_2 analytics.

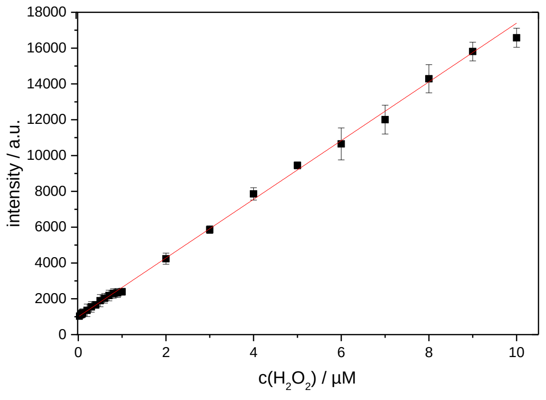


Figure S6. Calibration curve of H_2O_2 analytics.

1.3. Photocatalytic MB degradation with WLE

Table S2. Kinetic data for MB decolouration reactions.

n WLE	Photon flux density nE L^{-1} min^{-1}	k_D nM min^{-1}	ξ %
1	47818.2	8.5	0.0178
2	113991.7	17.7	0.0155
3	135260.3	22.6	0.0167
4	189011.4	25.9	0.0137
5	237270.3	29.9	0.0126

1.4. Photocatalytic NB reduction to AN with WLE

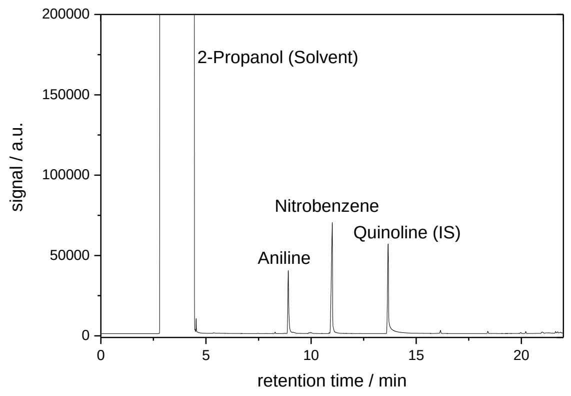


Figure S7. Exemplary GC spectrum after 5 h reaction time.

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Table S3. Kinetic data for NB reduction.

n WLE	Photon flux density mE L^{-1} h^{-1}	k_B (AN) mM min^{-1}	ξ_{AN}[1] %
5	14.2362	0.94	26

[1]assuming six photons for each conversation

1.5. Principal performance figures of the WLE

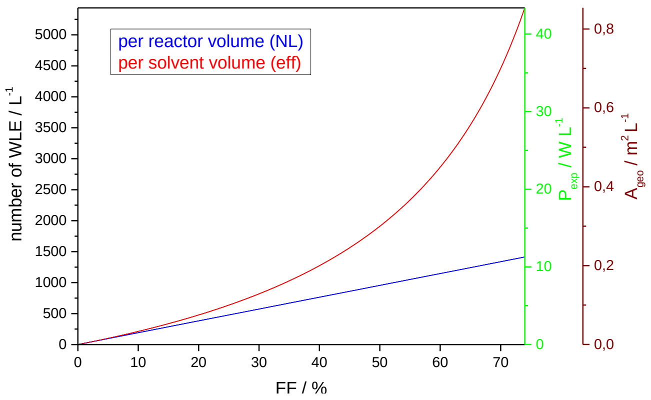

Figure S8. Principal performance figures of the WLE system in dependence of different densities of WLE / fill factors.

Calculation of the performance figures using volume of each WLE V_{WLE} = 0.52 mL, specific radiant power of each WLE P_{exp} = 0.08 W WLE^{-1}, specific surface area of each WLE (only counting the top half which is internally illuminated) $A_{1/2\ WLE}$ = 1.57 cm^2:

Number of WLE per reactor volume n_{WLE} (NL):

$$n_{WLE}(NL) = \frac{FF \times V}{V_{WLE}}$$

Number of WLE per effective reaction medium volume n_{WLE} (eff):

$$n_{WLE}(eff) = n_{WLE}(NL) \times \frac{1}{(1 - FF)}$$

Total radiant flux density per reactor volume P_{exp} (NL):

$$P_{exp}(NL) = n_{WLE}(NL) \times P_{WLE}$$

Total radiant flux density per effective reaction medium volume P_{exp} (eff):

$$P_{exp}(eff) = n_{WLE}(eff) \times P_{WLE}$$

Total photon flux densities were calculated from the radiant flux densities by multiplying them with 3,05 µE J^{-1} which is derived from the factor $N_A^{-1} \cdot h^{-1} \cdot c^{-1} \cdot \lambda$ using the Avogadro constant N_A, planck constant h, light speed c and wavelength of the photons λ (365 nm).

Total geometric catalyst surface per reactor volume A_{geo} (NL):

$$A_{geo}(NL) = n_{WLE}(NL) \times A_{\frac{1}{2}WLE}$$

Total geometric catalyst surface per effective reaction medium volume A_{geo} (eff):

$$A_{geo}(eff) = n_{WLE}(eff) \times A_{\frac{1}{2}WLE}$$

Space time yield STY was calculated by multiplying the photon flux density by 3600 s h^{-1}.

1.6. Cost evaluation and data of the used WLE

The main part for the cost of the used WLE is the UV-LED, *cf.* Table S4. A cost reduction and more efficient LEDs are expected soon according to Haitz´s law.[2] In comparison to the one year old used LED, already today cheaper and higher powered LEDs are available.[3] For example a 365 nm LED with comparable performance is now available for 3.97 € (also at a quantity of 100).[4] Further cost reductions can be achieved by raising the quantity and therefore lowering the fixed costs for fabrication considerably, at quantities of >1000 units, the fabrication costs drop well below 1 € per unit.

Table S4. Cost evaluation of the used WLE with an order quantity of 100 WLE.

part	Cost / € per WLE
mounted LED	26.39
fabrication of LED	3.90
COP (polymer shell, 0,25 g per shell)	0.02
fabrication of the shell	1.47
Sum	31.78

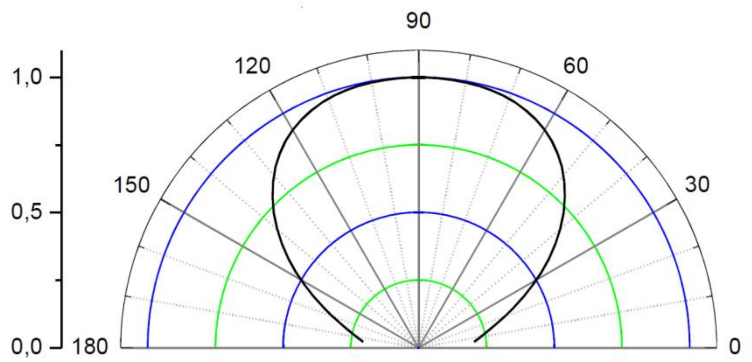

Figure S9. .View angle of the used LED (taken from the data sheet).

1.7. Power consumption and CO_2 footprint

The power consumption was measured as wall-plug-efficiency using a commercial power meter and found to be 8 W, invariant of the number of WLEs used (1 to 5). Using this power consumption, it is possible to calculate the energy consumption and CO_2 footprint of the reactions studied here, cf. Table S5. The table lists also an outlook at the efficiency of the system when it would be optimized to the state-of-the-art RIC and LED efficiencies. Also, the CO_2 footprint could be further lowered by using renewable energy sources. Nevertheless, the photonic efficiency of a reaction limits the overall efficiency of the system. Therefore reactions like H_2O_2 generation will remain rather inefficient and could be mainly enhanced developing more efficient catalysts.

Table S5. Calculation of power consumption and CO_2 footprint for H_2O_2 generation and NB reduction with 5 WLE.

Product	Energy consumption / kWh kg^{-1} product	CO_2 footprint / kg CO_2 kg^{-1} product[d]
Aniline[a]	10,308	5,432
Aniline[b]	4,569	2,408
Aniline[c]	86	45
H_2O_2[b]	968,289	510,288

[a] calculated with reaction data shown in Fig. 6 after 24 h.

[b] calculated with the respective formation rates.

[c] calculated for an optimized system with the assumption of 75% RIC efficiency and 35% LED efficiency.

[d] calculated with 527 g kWh^{-1}; value for the German electricity mix 2016.[5]

2. Notes and references

1 C. Kormann, D. W. Bahnemann and M. R. Hoffmann, *Environ. Sci. Technol.*, 1988, **22**, 798–806.

2 *Nat. Photonics*, 2007, **1**, 23–23.

3 M. Sender and D. Ziegenbalg, *Chemie Ing. Tech.*, 2017, 1–16.

4 Mouser Electronis, http://www.mouser.de/Optoelectronics/LED-Lighting/LED-Emitters/High-Power-LEDs-Single-Color/_/N-8usfn?P=1yzt848Z1z0z7pt, 11.07.2017.

5 Umweltbundesamt, 2017.

3. Author Contributions

B.O.B. and J.Z.B. and designed the experiments. B.O.B. carried out the coating procedures, characterisation and photocatalytic experiments. B.O.B. and J.Z.B. analysed the data and co-wrote the manuscript. A.S. designed the WLE's electronic circuit and the field generator for powering them. D.W.B. and J.Z.B. supervised the project. J.Z.B. conceived the concept.