Electronic Supplementary Material (ESI) for RSC Advances.
This journal is © The Royal Society of Chemistry 2016

Supporting Information

Immobilisation of Water-oxidising Amphiphilic Ruthenium Complexes on Unmodified Silica Gel

A. Králík, M. Hansen and B. König

Institute of Organic Chemistry, University of Regensburg, D-93040 Regensburg, Germany. E-mail: burkhard.koenig@ur.de

Table of Contents

General Methods and Material 2
Spectral Data 2
Heterogeneous Photocatalytic Water Oxidation
Summarised Experimental Data 4
Reactivation 5
Heterogeneous Photocatalytic Water Oxidation
Summarised Experimental Data 5

General Methods and Material

Fibox 3 fibre optic oxygen sensor (PreSens GmbH) was used for *in situ* monitoring of the oxygen evolution.

Head-space GC measurements were carried out on Inficon Micro GC 3000 with a 3 Å molecular sieve column, a thermal conductivity detector and argon as a carrier gas.

UV-VIS spectra were measured on Varian Cary 50 Bio UV-Visible.

For the visible light irradiation, OSRAM Oslon SSL 80 royal-blue LEDs were used.

Macherey-Nagel brand silica gels with 60 Å pore size and particle sizes of 63–200 or 40–63 µm were used for immobilisation.

Photosensitisers **1a**[1] and **1b**,[2] and catalysts **2a**,[3] **2b**[2] and **3**[4] were prepared according to literature procedures. Other commercially available chemicals were used without further purification.

Spectral Data

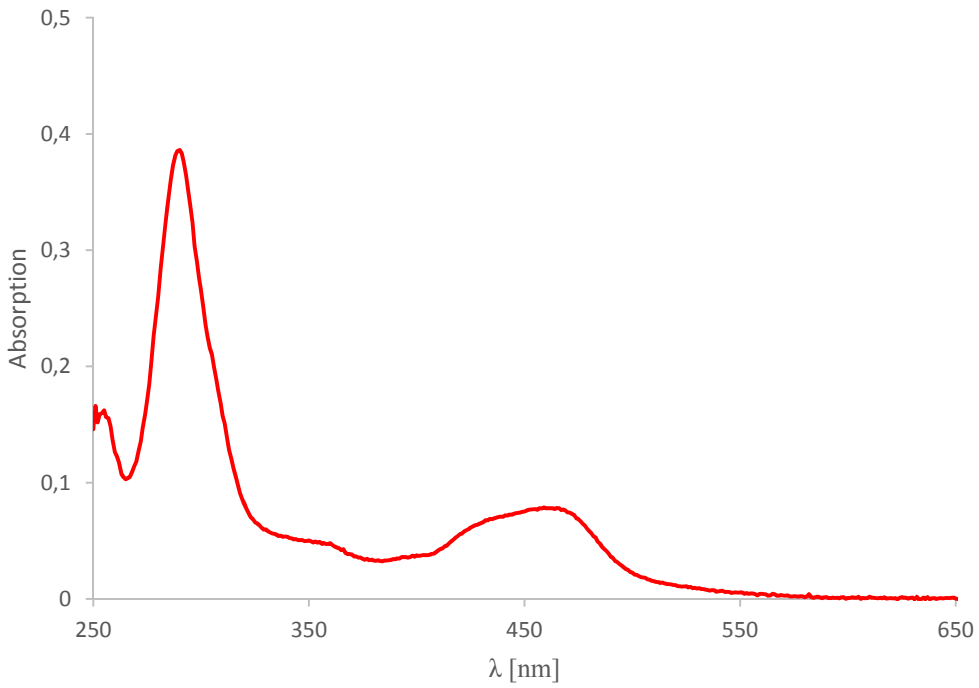

Figure S1: UV-VIS spectrum of 5 µM chloroform solution of photosensitiser **1b**.

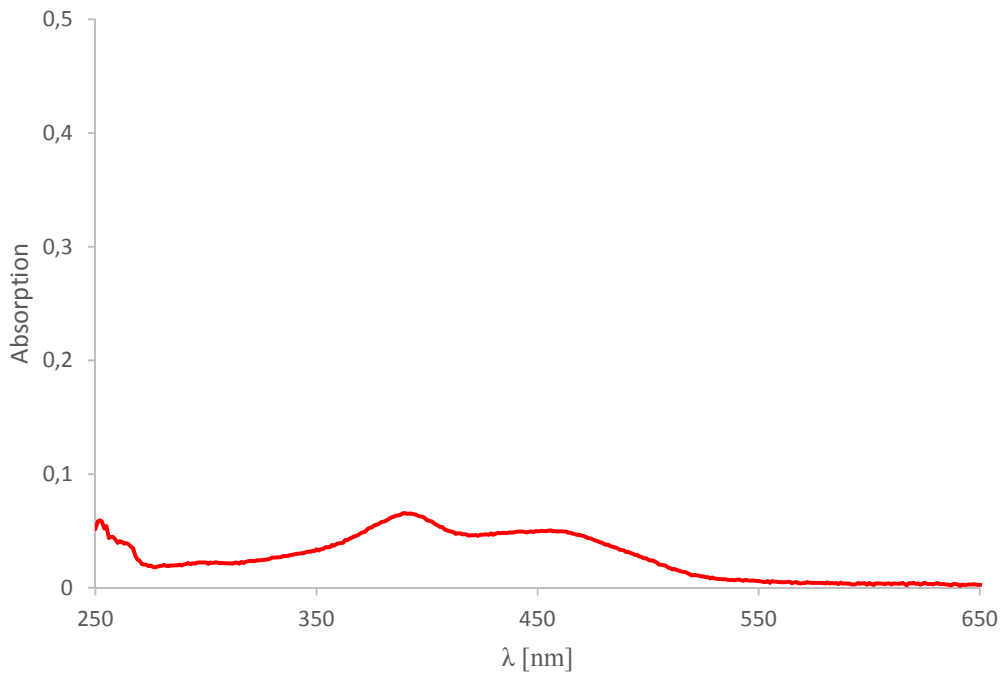

Figure S2: UV-VIS spectrum of 5 µM chloroform solution of catalyst **2b**.

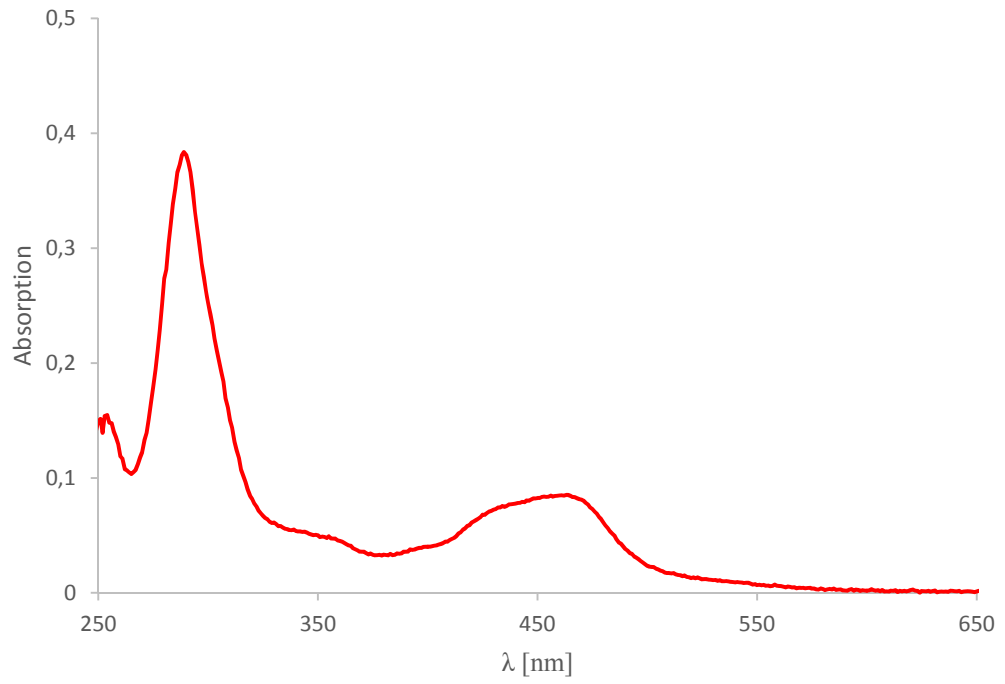

Figure S3: UV-VIS spectrum of chloroform solution containing photosensitiser **1b** (5 µM) and catalyst **2b** (0.5 µM).

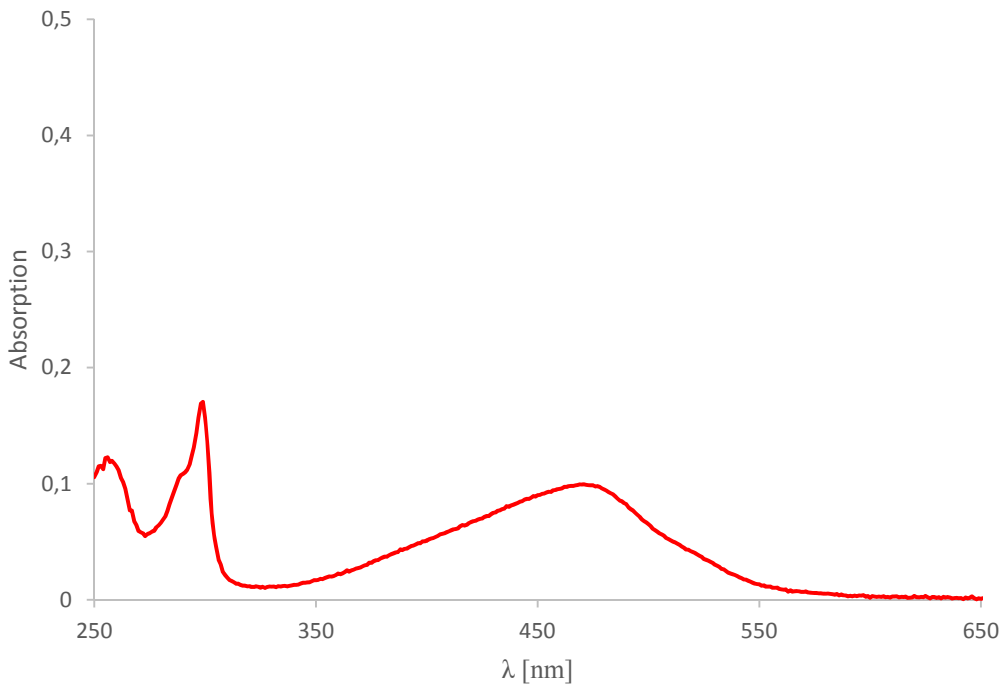

Figure S4: UV-VIS spectrum of 5 µM chloroform solution of catalyst **3**.

Heterogeneous Photocatalytic Water Oxidation

Summarised Experimental Data

Entry	Loading of 1b [µmol/g]	Loading of 2b [µmol/g]	PS:Cat ratio	Amount of SiO_2 [mg]	Amount of 1b [µmol]	Amount of 2b [µmol]	Evolved oxygen [µmol]	TON
1	20	2	10:1	30[a]	0.6	0.06	2.8	48
2	10	1	10:1	60[a]	0.6	0.06	2.1	34
3	5	0.5	10:1	120[a]	0.6	0.06	3.2	53
4	2	0.2	10:1	300[a]	0.6	0.06	2.6	42
5	20	2	10:1	30[b]	0.6	0.06	2.5	41
6	10	1	10:1	60[b]	0.6	0.06	1.8	30

[a] particle size 63–200 µm; [b] particle size 40–63 µm

Reactivation

Entry	Loading of 1b [µmol/g]	Loading of 2b [µmol/g]	PS:Cat ratio	Amount of SiO_2 [mg]	Amount of 1b [µmol]	Amount of 2b [µmol]	Evolved oxygen [µmol]	TON
1	20	2	10:1	30	0.6	0.06	2.8	48
2	20[a]	2[b]	10[a]:1[b]	30[c]	0.6[a]	0.06[b]	2.4	40

[a] fresh batch of photosensitiser; [b] leftover catalyst from previous water oxidation reaction; [c] silica gel recovered from entry 1

Heterogeneous Chemical Water Oxidation

Summarised Experimental Data

Entry	Loading of 3 [µmol/g]	Amount of SiO_2 [mg]	Amount of 1b [nmol]	Evolved oxygen [µmol]	TON
1[a]	-	-	4	0.16	41 000
2	2	2	4	0.11	29 000
3	1	4	4	0.09	24 000
4	0.5	8	4	0.10	26 000
5	0.2	20	4	0.07	17 000
6	0.1	40	4	0.10	25 000

[a] homogeneous experiment

References

1. H. Xia, Y. Zhu, D. Lu, M. Li, C. Zhang, B. Yang and Y. Ma, *J. Phys. Chem. B*, 2006, **110**, 18718-18723.
2. M. Hansen, F. Li, L. Sun and B. Konig, *Chem. Sci.*, 2014, **5**, 2683-2687.
3. L. Duan, Y. Xu, M. Gorlov, L. Tong, S. Andersson and L. Sun, *Chem. Eur. J.*, 2010, **16**, 4659-4668.
4. L. Wang, L. Duan, Y. Wang, M. S. G. Ahlquist and L. Sun, *Chem. Commun.*, 2014, **50**, 12947-12950.