

## **[Ru<sup>V</sup>(NCN-Me)(bpy)(=O)]<sup>3+</sup> Mediated Efficient Photo-driven Water Oxidation**

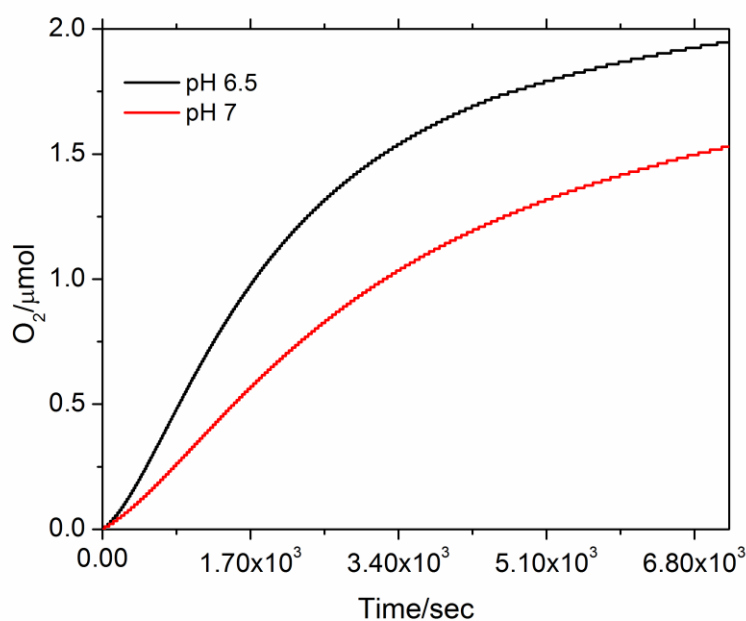
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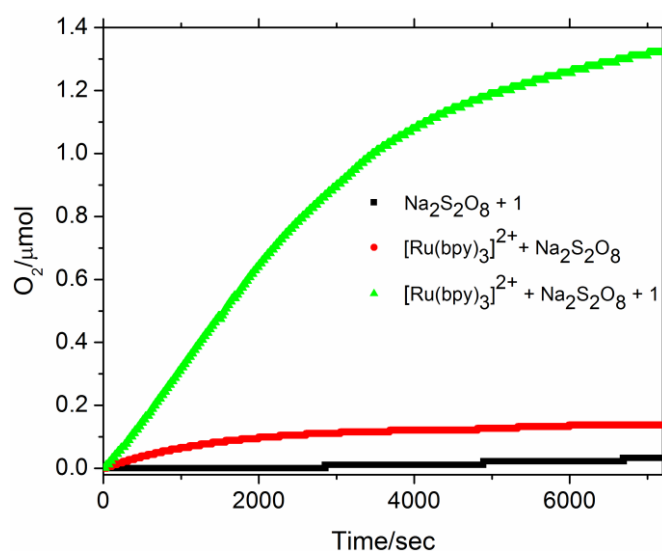
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**Supporting Information**

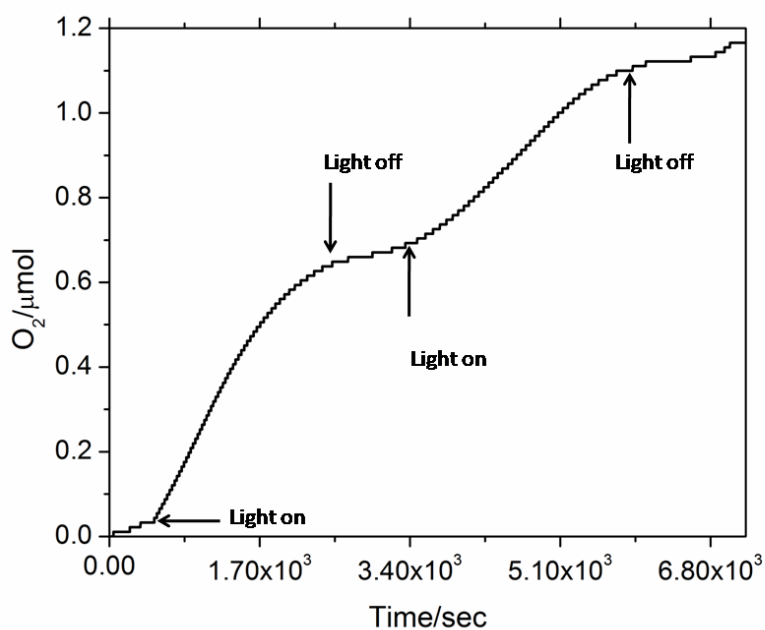
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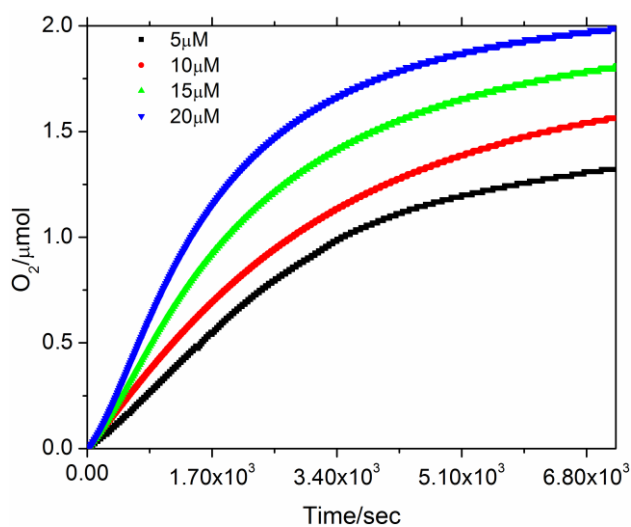
**Figure S1.** Photochemical  $O_2$  evolution in 2 mL of phosphate buffer solution at two different pH (7 and 6.5) containing  $Na_2S_2O_8$  ( $1 \times 10^{-2}$  M),  $[Ru(bpy)_3]Cl_2$  ( $1 \times 10^{-3}$  M) and  $[Ru(NCN-Me)(bpy)(OH_2)](PF_6)_2$  ( $5 \times 10^{-7}$  M).



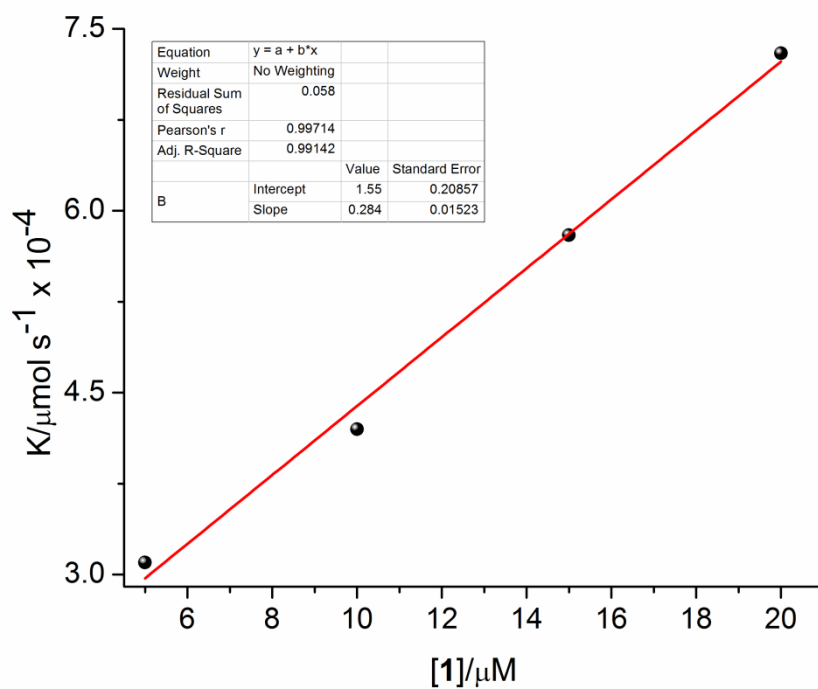
**Figure S2.** Photochemical oxygen evolution in phosphate buffer solution (pH=6.47, 2mL) of (a)  $Na_2S_2O_8$  ( $1 \times 10^{-2}$  M) and catalyst  $[Ru(NCN-Me)(bpy)(OH_2)](PF_6)_2$  (**1**) ( $5 \times 10^{-6}$  M) black curve (b)  $Na_2S_2O_8$  ( $1 \times 10^{-2}$  M)  $[Ru(bpy)_3]Cl_2$  ( $1 \times 10^{-3}$  M), red curve (c)  $Na_2S_2O_8$  ( $1 \times 10^{-2}$  M),  $[Ru(bpy)_3]Cl_2$  ( $1 \times 10^{-3}$  M), catalyst  $[Ru(NCN-Me)(bpy)(OH_2)](PF_6)_2$  (**1**) ( $5 \times 10^{-6}$  M), green curve.



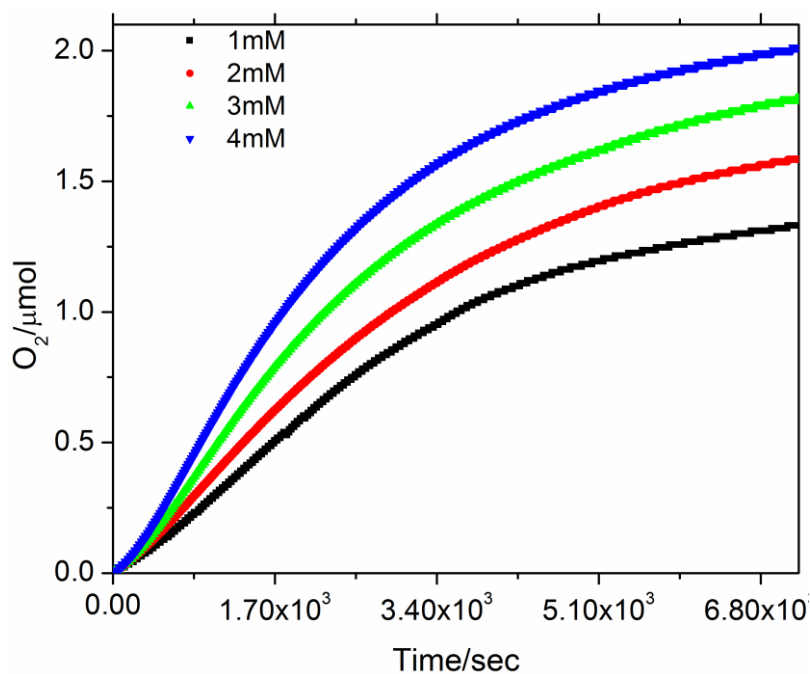
**Figure S3.** Light control experiment of the photochemical water oxidation in a phosphate buffer solution (2mL, pH=6.5) of  $[\text{Ru}(\text{bpy})_3]\text{Cl}_2$  ( $1 \times 10^{-3} \text{ M}$ ),  $\text{Na}_2\text{S}_2\text{O}_8$  ( $1 \times 10^{-2} \text{ M}$ ) and catalyst  $[\text{Ru}(\text{NCN-Me})(\text{bpy})(\text{OH}_2)](\text{PF}_6)_2$  (**1**) ( $5 \times 10^{-6} \text{ M}$ ).



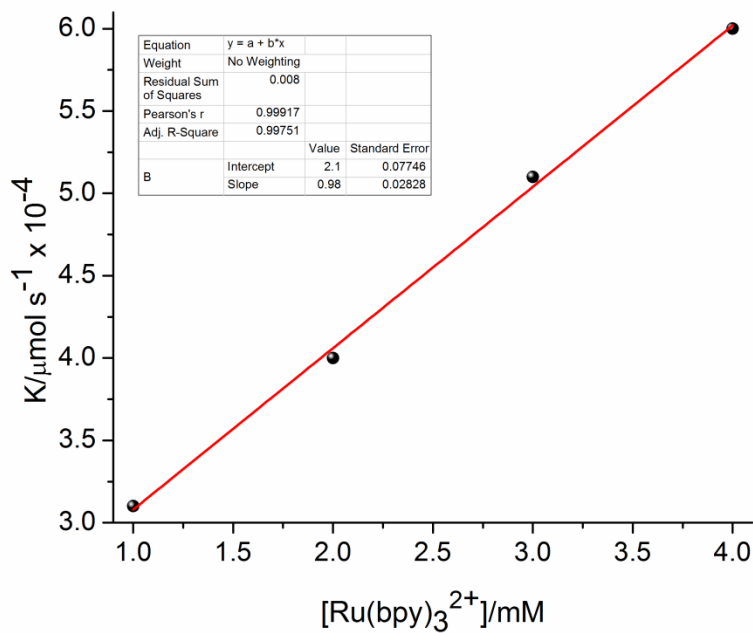
**Figure S4.**  $\text{O}_2$  evolution at pH 6.5 in phosphate buffer having  $\text{Na}_2\text{S}_2\text{O}_8$  ( $1 \times 10^{-2} \text{ M}$ ),  $[\text{Ru}(\text{bpy})_3]\text{Cl}_2$  ( $1 \times 10^{-3} \text{ M}$ ) with various concentration of **1**.



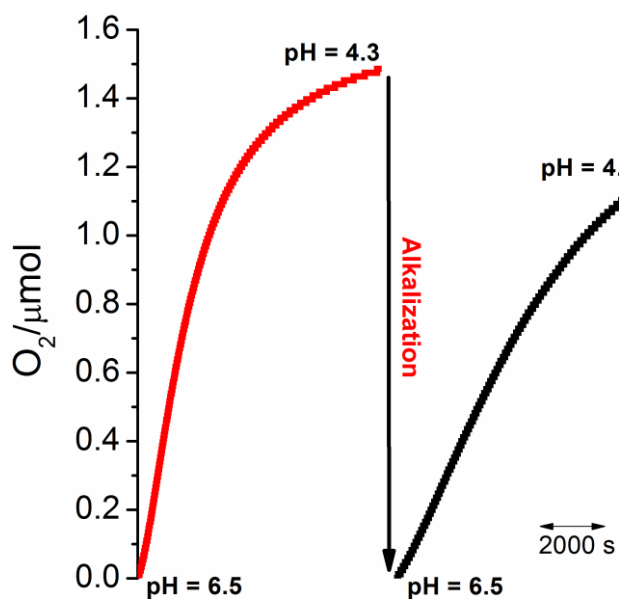
**Figure S5.** Rate of O<sub>2</sub> evolution with varied concentration of catalyst [Ru(NCN-Me)(bpy)(OH<sub>2</sub>)](PF<sub>6</sub>)<sub>2</sub> (**1**) in phosphate buffer pH-6.5.



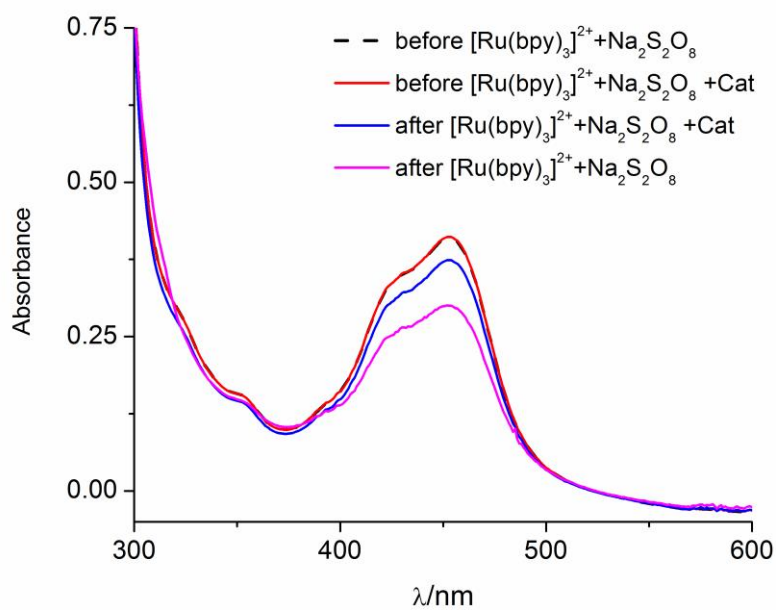
**Figure S6.** O<sub>2</sub> evolution by 5 μM of [Ru<sup>II</sup>(NCN-Me)(bpy)(OH<sub>2</sub>)]<sup>2+</sup> (**1**) in phosphate buffer (2mL, pH= 6.5), Na<sub>2</sub>S<sub>2</sub>O<sub>8</sub> (1 x 10<sup>-2</sup>M) and various concentration of [Ru(bpy)<sub>3</sub>]Cl<sub>2</sub>.



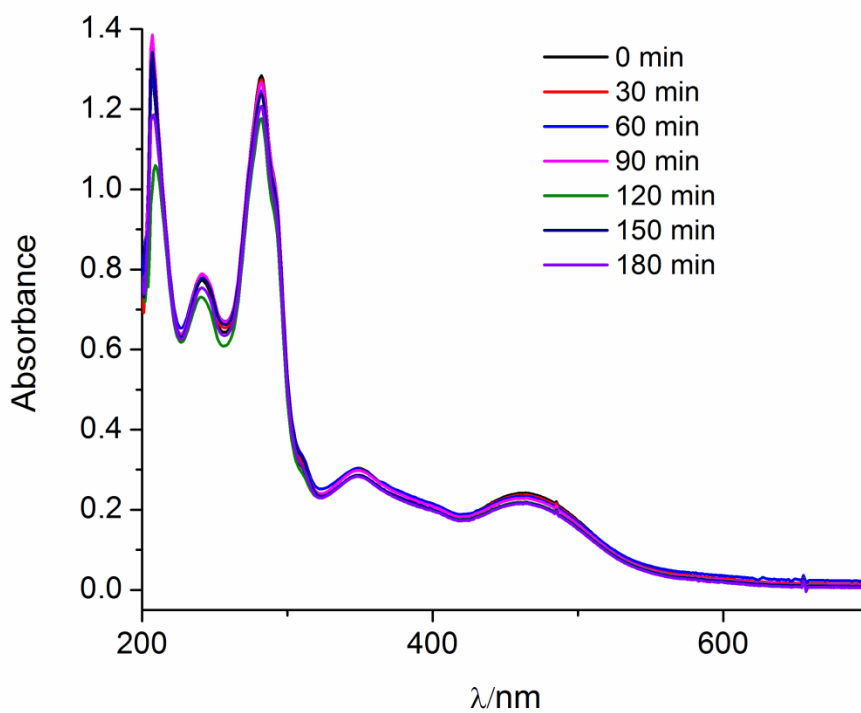
**Figure S7.** Rate of O<sub>2</sub> evolution by catalyst [Ru<sup>II</sup>(NCN-Me)(bpy)(OH<sub>2</sub>)]<sup>2+</sup> (**1**) (5 × 10<sup>-6</sup> M) with various concentration of [Ru(bpy)<sub>3</sub>]Cl<sub>2</sub>.



**Figure S8.** O<sub>2</sub> evolution in phosphate buffer (2 mL, pH=6.5) containing Na<sub>2</sub>S<sub>2</sub>O<sub>8</sub> (1 × 10<sup>-2</sup> M), [Ru(bpy)<sub>3</sub>]Cl<sub>2</sub> (1 × 10<sup>-3</sup> M) catalyst **1** (10 × 10<sup>-6</sup> M) and its successive reactivation of a photochemical water oxidation system by alkalization.



**Figure S9.** Absorption spectral changes of solutions before and after irradiation.



**Figure S10.** Absorbance-time traces of 20 μM catalyst [Ru(NCN-Me)(bpy)(OH<sub>2</sub>)](PF<sub>6</sub>)<sub>2</sub> (**1**) in a phosphate buffer (pH-6.5) upon visible light irradiation.