

Robotic optimization of photocatalytic water oxidation

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A robotic setup for photocatalytic water oxidation has been developed, using a Chemspeed synthesis platform. In it, the entire reaction workflow is automated, ranging from reagent dosing, degassing, light source control and *in situ* monitoring of oxygen evolution. As a model system for photocatalytic water oxidation [Ru(bpy)₃]Cl₂ was chosen as photosensitizer and catalyst along with sodium persulfate as sacrificial electron acceptor.^[1] Based on this reaction set-up, we are investigating the influence of the [Ru(bpy)₃]Cl₂ concentration, different sacrificial electron acceptors and their concentration, different pH values and different light intensities as well as irradiation wavelengths. After generating a basic parameter space for these variables, the further optimization is done utilizing machine learning (Gaussian process regression) in a closed loop optimization. With this we establish a new automated setup for the investigation of water oxidation catalysts and in the future also for overall water splitting systems.

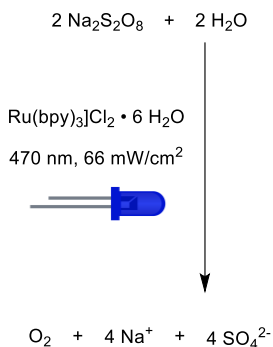
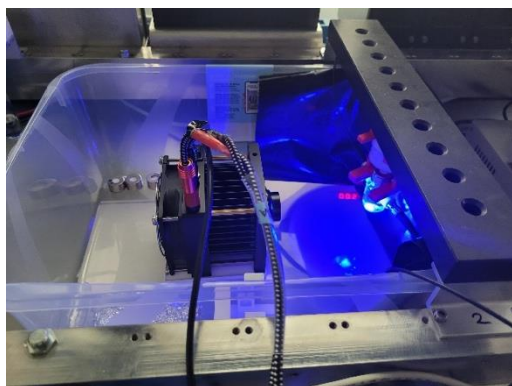


Figure 1: Left: Irradiation setup in a Chemspeed robot, with the 470 nm light source on the left and the reaction vessel on the right.^[2] Right: reaction equation of the water oxidation reaction.

[1] U. S. Akthar *et al.*, ACS Catal., 2016, **6**, 8361, 10.1021/acscatal.6b02595

[2] Foto: M. Ringleb