



WORKSHOP ON NEW MATERIALS FOR RENEWABLE ENERGY
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Ru BASED WATER OXIDATION CATALYSTS

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ABSTRACT II:

Oxygen-Oxygen bond formation is the key step for the oxidation of water to molecular oxygen: a reaction of interest from a biological perspective and also for establishing new energy conversion schemes. A few Ru complexes have been described recently that are capable of catalyzing the water oxidation reaction, and their performance has been shown to be strongly dependent on, nuclearity, oxidation state and ligand topology.^[1]

A step forward in the field consists on unraveling the different reaction pathways through which these reactions proceed. We have tackled this challenging topic by carrying out thorough electrochemical, spectroscopic and kinetic analysis together with O-18 labeling studies and DFT calculations. The combination of all these results gives evidence for mechanisms involving: intramolecular O-O bond formation, water nucleophilic attack and bimolecular O-O bond formation.^[2]

The anchoring of these catalysts into conducting solid supports is therefore the next mandatory step to demonstrate the feasibility of building a solid-state device for water oxidation that could be integrated into a larger device for the photo-production of H₂. Polypyrrolic electro-polymerization onto vitreous carbon sponges (VCS) and fluorine-doped tin oxide (FTO), and anchoring onto rutile TiO₂ or FTO-TiO₂ surfaces have been the explored strategies. The catalytic performance of these new heterogeneous water oxidation systems will also be discussed.^[3]

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